vibrational peak at 70 meV are less affected than in the Vycor case. However, an up-shift of the librational peak at 70 meV, characteristic of hindered motions, is observed (50).

Biopolymer-Water Systems

The volume of neutron data on biopolymer-water systems has increased during the past years (60,82,83). The situation is more complex because of contributions such as the hydrogen atoms of the protein itself, the possibility of their exchange with water molecules, and the presence of hydrophilic and hydrophobic regions. The studies of single-particle dynamics of hydration water in proteins have been hampered by the fact that about 40% of the constituent atoms in a typical protein molecule are hydrogen atoms, present in the backbone and side chains. The elastic contribution is thus too large for an accurate determination of the dynamical parameters which are characteristic of hydration process. However, by working with a deuterated protein/H_2O system, it has been possible recently to focus on the water dynamics at and near the protein surface (57–59).

At the vicinity of biomolecules, water may adopt very different behaviors depending on the nature of the sites, available free volume, temperature, etc. Because of the difficulty of experiments that can identify local properties among a variety of possibilities, the number of unambiguous results remains scarce. It is plausible that the development of computer simulations of molecular dynamics soon will take into account local environments more precisely (39–41).

Quasi-elastic neutron scattering has been used to describe the motions of water molecules in the vicinity of proteins and other macromolecules. One of the more successful results has been obtained with C-phycocyanin, a protein extracted from blue-green algae, which can be obtained nearly fully deuterated from perdeuterated cultures as mentioned previously (56). In this way, and because of the very large incoherent cross-section of hydrogen atoms, only the motions of water molecules are observed in a quasi-elastic neutron-scattering experiment (57–59). The results presented in Figure 7 show clearly that the total scattered intensity contains two components. The width of the narrow component is imposed by the instrumental resolution. Its area is proportional to the number of water molecules with motions that are too slow to be observed by the technique, that is, typically with a characteristic time longer than several tens of picoseconds. Instead, the wider component depicts the diffusive motions of the other water molecules through a Lorentzian line $L(\omega)$. Its intensity and width can be analyzed as functions of the degree of hydration and of temperature.

The simplest expression that can be written separates the two components in the following way:

$$S_{\text{inc}}(Q,\omega) = [P + (1-P)A_0]\delta(\omega) + (1-P)(1-A_0)L(\omega) \qquad (2)$$

where $P = p + q(1-p)$ contains both the contributions of the p nonlabile protons of the protein and the fraction q of water molecules with a slow dynamics. A_0(Qa) is a mathematical factor, called *elastic incoherent scattering factor*, which takes into account the confinement of the motions within a small volume of size a, assumed spherical for simplicity (80).

Typical results are shown in Figure 8. Figure 8A shows that the number q of "immobile" water molecules increases gradually from 40%, at high temperature, to 100% at around 200 K. This result shows that the number of confined