Quasielastic spectra in the Mössbauer effect and neutron scattering

Hans Frauenfelder, Robert D. Young, and Paul W. Fenimore

Los Alamos National Laboratory and Center for Biological Physics, Arizona State University, USA

In proteins the Mössbauer effect and neutron scattering show a rapid increase of the mean-square-displacement (msd) above about 180 K. The increase is accompanied by the appearance of a broad band. The standard explanation of the increase, dubbed "dynamical transition", is controversial and no satisfactory explanation for the broad band has been put forward. We introduce a new interpretation of the Mössbauer effect in proteins. We prove that there is no dynamical transition and that the separation into a sharp line and a broad band is misleading. The broad band is inhomogeneous and is composed of sharp Mössbauer lines that have been shifted by βh fluctuations in the protein's hydration shell and α fluctuations in the bulk solvent. In the crystals used for the Mössbauer experiments the α fluctuations are absent. Using the dielectric spectrum of the βh fluctuations, we predict the shape of the Mössbauer spectrum from 80 K to 295 K with one dimensionless coefficient. The explanation is important for the dynamics of proteins and for the interpretation of quasielastic neutron scattering in complex systems.