The temperature, angle and energy dependent dynamics of a protein investigated by phonon assisted Mössbauer effect and Mössbauer absorption

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The structure and the dynamics of proteins is governed by a wide spectrum of interactions: covalent bonds, H-bridges, Coulomb- , van der Waals- and hydrophobic interactions. The protein structure can be determined by X-ray structure analysis in great detail. In order to investigate the physics of protein dynamics many experimental and theoretical methods are necessary. In the following we discuss investigations on myoglobin which stores O_2 and regulates the NO concentration in the cell.

The phonon assisted Mössbauer effect is used to investigate the harmonic vibrations of myoglobin in the meV energy regime. The neV energy region is covered by Mössbauer absorption experiments. The natural iron in the active center is replaced by the Mössbauer isotope ^{57}Fe and applied as a label for this motions. A single crystal of metmyoglobin, with $P2_1$ symmetry, is explored in 5 different orientations around the crystallographic b-axes. The phonon spectra between ±80meV show clear orientation dependencies hence the method is sensitive to the projection of the vibrational amplitude onto the beam directions. About 10 groups of modes (heme sliding motions, vibrations within the heme plane and perpendicular to the plane) can be identified by a pronounced orientation dependence. The density of phonons below 1meV is due to acoustic phonon modes and shows a quadratically increase with the energy like in a Debye solid. An anisotropic velocity of sound in the protein crystal is extracted from the quadratic slope below 1meV with a mean sound velocity of 1657 m/s. A Debye-like behavior is extended to about 3meV into the optical phonon energy regime without an energy gap or a signature of van Hove singularities. Temperature dependent measurements on a huge number of small crystals and on amorphous samples show that the density of states is temperature independent also in the physiological temperature regime above 180K. The temperature dependent mean square displacement due to harmonic vibrations between 40K and 300K can be subdivided into three parts: ~20% is due to acoustic like modes in the Debye regime, ~40% is due to modes showing a Debye-like dispersion, the rest of ~40% is due to true optical modes. The mean square displacements obtained by the phonon assisted Mössbauer effect can be compared with Mössbauer absorption experiments: the protein specific, functional important dynamics reveals itself in the Mössbauer absorption experiment as quasielastic broad lines not extending into the meV energy region. There seems to be an energy (or time) gap between the solid state vibrations and the protein specific motions, becoming active above a dynamical transition temperature. The presented results confirm that the solid state vibrations stay harmonic up to physiological temperatures. The direction and amplitude of the identified modes can be used to refine the potential functions used in normal mode calculations. Corresponding computations using CHARMM are in progress. A comparison with a neutron structure analysis of myoglobin shows, that the iron motion represents the backbone motion of the protein whereas inelastic neutron scattering experiments are sensitive mainly to side chain motions.