The Onset of Collective Structural Vibrations at the Protein Dynamical Transition

MENGYANG XU, KATHERINE A. NIESSEN, YANTING DENG, NIGEL S. MICHIKI, State Univ of NY - Buffalo, Buffalo, NY, EDWARD H. SNELL, Hauptman-Woodward Medical Research Institute, State Univ of NY - Buffalo, Buffalo, NY, ANDREA G. MARKEIZ, State Univ of NY - Buffalo, Buffalo, NY — X-ray, neutron scattering and terahertz measurements [1,2] found a rapid increase in dynamics of critically hydrated proteins above 220 K, termed the protein dynamical transition. Protein function ceases below the DT. It has been suggested that protein dynamics is slaved to the solvent and the DT originates from thermally activated solvent motions. Since previous measurements did not distinguish local diffusive and librational motions from long-range collective vibrations of proteins, it has not been determined how long-range motions are affected by the DT. Using a recently developed technique, crystal anisotropy terahertz microscopy [3] we directly measured the long-range motions for lysozyme and examined the temperature dependence in the 180-290 K range. We find that the distinct intramolecular vibrations do not follow the expected phonon-like behavior of solid state systems where the vibrational bands sharpen and blue shift with decreasing temperature, rather decrease in intensity as the DT is approached and disappear below the DT. This suggests the surrounding solvent below the DT acts as a frozen cage preventing long-range motions. 1. Doster, W., et al. Phys. Rev. Lett., 2010.104(9):098101. 2. Niessen, K., et al. Biophys. Rev., 2015.7,201. 3. Acbas, G., et al. Nat. Commun., 2014.5,3076.

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