



The Physics of Soft and Biological Matter

P.32 Hydration dynamics of proteins in solutions studied in 220-325 GHz band

O Sushko, R Dubrovka and R Donnan

School of Electronic Engineering and Computer Science, Queen Mary University of London, UK

The transmission measurements of protein water solutions have been performed using a vector network analyser-driven quasi-optical bench covering the waveguide band 220-325 GHz. The following proteins, ranging from lower to higher molecular weight, were chosen for this study: lysozyme, myoglobin and bovine serum albumin (BSA). A special liquid cell with TPX windows and 100 μm window separation (spacer) have been used to study these. Defined amounts of each protein were dissolved in distilled water without adding any salt-buffer. Absorption properties of solutions were studied at different concentrations ranging from 2 to 100 mg/ml. The molecular dynamics simulator Gromacs was used to accurately estimate the number of water molecules excluded by each protein. The initial purpose is to check whether all protein solutions consistently exhibit a decreased absorption compared to bulk water (THz defect) in the lower THz spectral domain (0.22 – 0.325 THz). A THz defect was the expected scenario, since protein molecules have far less absorption than water molecules. However at low protein concentration the recorded spectra showed an initial rise or a plateau in absorption compared to bulk water (THz excess) followed by a decrease in absorption. This non-linear trend in solution absorption was consistently observed for all three proteins. According to our findings, this point of inflection is not related to the onset of the protein hydration shells overlap, since it occurs at rather dilute concentrations. Instead, the results suggest that the molar protein absorption in solution is significantly higher compared dry-state protein. This effect is especially evident at low protein concentrations of about 10-20 mg/ml. Previously THz excess of protein solutions has been reported only at frequencies above 2 THz. The data obtained shows that three different protein solutions consistently exhibit THz excess in the lower THz domain considered. This in turn suggests that protein water interaction is more complex than previously believed.