SUB-TERRAHERTZ SPECTROSCOPY OF E.COLI DNA: EXPERIMENT, STATISTICAL MODEL, AND MD SIMULATIONS

I. SIZOV, T. DOROFEEVA, T. KHROMOVA, B. GELMONT, and T. GLOBUS, *Department of Electrical and Computer Engineering, University of Virginia, Charlottesville, VA 22904*.

We will present result of combined experimental and computational study of sub-THz absorption spectra from *Escherichia coli* (*E.coli*) DNA. Measurements were conducted using a Bruker FTIR spectrometer with a liquid helium cooled bolometer and a recently developed frequency domain sensor operating at room temperature, with spectral resolution of 0.25 cm^{-1} and 0.03 cm^{-1}, correspondingly. We have earlier demonstrated that molecular dynamics (MD) simulation can be effectively applied for characterizing relatively small biological molecules, such as transfer RNA or small protein thioredoxin from *E. coli* , and help to understand and predict their absorption spectra. Large size of DNA macromolecules (5 million base pairs for *E. coli* DNA) prevents, however, direct application of MD simulation at the current level of computational capabilities. Therefore, by applying a second order Markov chain approach and Monte-Carlo technique, we have developed a new statistical model to construct DNA sequences from biological cells. These short representative sequences (20-60 base pairs) are built upon the most frequently repeated fragments (2-10 base pairs) in the original DNA. Using this new approach, we constructed DNA sequences for several non-pathogenic strains of *E.coli*, including a well-known strain BL21, uro-pathogenic strain, CFT073, and deadly EDL933 strain (O157:H7), and used MD simulations to calculate vibrational absorption spectra of these strains. Significant differences are clearly present in spectra of strains in averaged spectra and in all components for particular orientations. The mechanism of interaction of THz radiation with a biological molecule is studied by analyzing dynamics of atoms and correlation of local vibrations in the modeled molecule. Simulated THz vibrational spectra of DNA are compared with experimental results. With the spectral resolution of 0.1 cm^{-1} or better, which is now available in experiments, the very easy discrimination between different strains of the same bacteria becomes possible.