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Higher order structure of macromolecules studied by Terahertz spectroscopy

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Recent rapid development of spectroscopic techniques in terahertz (THz) frequency region enables rapid and precise measurement of low-frequency molecular vibrations. Since information about intermolecular structure and interactions (rather than intramolecular structure) can be obtained from THz spectra, it will become a powerful tool for monitoring higher order conformations of macromolecules. Recently, we have measured the THz spectra of poly(3-hydroxybutyrate) (PHB) and found clear differences between the spectrum of amorphous PHB and that of crystalline PHB. Using polarization spectroscopy, the vibrational peaks of crystalline PHB corresponding to the skeletal vibration of the helical structure and the vibration between helical structures could be assigned. Furthermore, we have developed method for spectral calculation based on DFT.

Spectroscopic information in THz frequencies help to understand conformational change of macromolecules. We observed the isothermal crystallization of PHB by monitoring the temporal evolution of terahertz absorption spectra in conjunction with spectral analysis using two-dimensional correlation spectroscopy. We have also observed the Brill transition of Nylon-6 by temperature dependent absorption spectra.

Thus THz spectroscopy represents a useful technique for unearthing information about polymer structures, and this technique has the potential to become a powerful tool for polymer science.

Biography

Hiromichi Hoshina received BS degree in 1998, MS degree in 2000 and PhD in 2003 from Kyoto University, Kyoto, Japan. From 2000, he was a Research Fellow of Japan Society for the Promotion of Science, and then moved to the Department of Chemistry, University of Southern California, Los Angeles, USA, as a Research Scholar in 2003. In 2005, he joined RIKEN as a Research Scientist. His current research interest is the molecular spectroscopy and imaging applications in terahertz frequency region.

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