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Title:Temperature and hydration dependence of low-frequency spectra of poly-l-glutamic acid with different secondary structures studied by terahertz time-domain spectroscopy
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Abstract:We have investigated low-frequency spectra of poly-l-glutamic acid (polyE) in the powder state by terahertz time-domain spectroscopy (THz-TDS). Samples with three different secondary structures (α-helix, β-sheet, and random-coil) and different chain lengths were prepared to investigate the dependence of the THz spectra on temperature and hydration. The temperature dependence of the THz absorption spectra clearly shows that polyE, regardless of its secondary structure, undergoes dynamical transition between 190 and 240 K. We have estimated the apparent activation energy and transition temperature by phenomenological spectral analysis. We also have estimated the effective dipole moment of the amino acid residue from the real part of the dielectric permittivity at zero frequency. Both results show that the transition temperature is lower when the secondary structure undergoes a transition from a random-coil structure to an α-helix or β-sheet structure. Furthermore, both hydrating water molecules and peptide hydrogen bonds contribute to induce anharmonicity in the low-frequency vibrational motions. Meanwhile, hydration, not peptide hydrogen bonds, is crucial for the dynamical transition to occur because the onset of anharmonicity was observed only when the polypeptide is hydrated. An apparent intermolecular vibrational mode in the β-sheet structure, which suggests a highly ordered structure in the sample, did not exhibit anharmonicity at the tested temperatures and humidity levels. This result suggests that short-range or inter-strand hydrogen bonds of the α-helix or low-ordered β-sheet structures gave rise to the lower transition temperatures and the smaller effective activation energies compared with those of the random-coil

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