Terahertz Dynamics of Electrolytes in Aqueous Biological Media

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We measured the dynamics of aqueous biomaterial mixtures using terahertz time-domain spectroscopy. The mixtures were divided into water and other electrolyte parts in mass fractions for analysis. The optical constants of the electrolytes, excluding water, were obtained by applying the ideal mixture equation and fitted with the modified double Debye model. We found that the reorientation and hydrogen-bond formation-decomposition times decreased as the electrolyte concentration increased.

I. INTRODUCTION AND BACKGROUND

The study of cells and proteins in the terahertz (THz) spectral region is important in acquiring information on bio-molecular conformational states. This is because the modes of twisting, bending, and folding motions in the conformation are distributed around a few THz. Various difficulties can arise in studying biomaterials in this region. One such difficulty is that the samples in the water heavily absorb the electromagnetic waves. It is also hard to determine the exact concentration as a mole or volume fraction of the biomaterials extracted naturally from a living body.

The Luria–Bertani (LB) medium studied in this work is conventionally used as the medium for culturing some bacteria, such as Escherichia coli (E. coli). The biomaterial properties can be characterized by complex optical and electrical constants dependent on the concentration in the THz region. THz time-domain spectroscopy (THz-TDS) is an excellent tool for studying the carrier or ion dynamics of semiconductors, electrolytes, and multiple mixtures. In this study, we measured the optical constants of biomaterial mixtures using THz-TDS, and extracted properties of electrolytes using mass fractions. The measurement results were fitted with a modified double Debye model to explain the ultrafast molecular dynamics of electrolytes.

II. RESULTS

We measured the optical constants of water and LB media by THz-TDS[1]. The LB media is the composite of sodium chloride and natural substances such as trypton and yeast extract for culturing certain bacteria.

Figs. 1(a) and (b) show the real and imaginary parts of the index of refraction, respectively. The index of refraction increased as the concentration of ingredients increased, implying that the index of refraction of biomaterials is larger than that of pure water. The imaginary part of the index of refraction decreased as the frequency increased, and crossed between 1.0 and 1.3 THz.

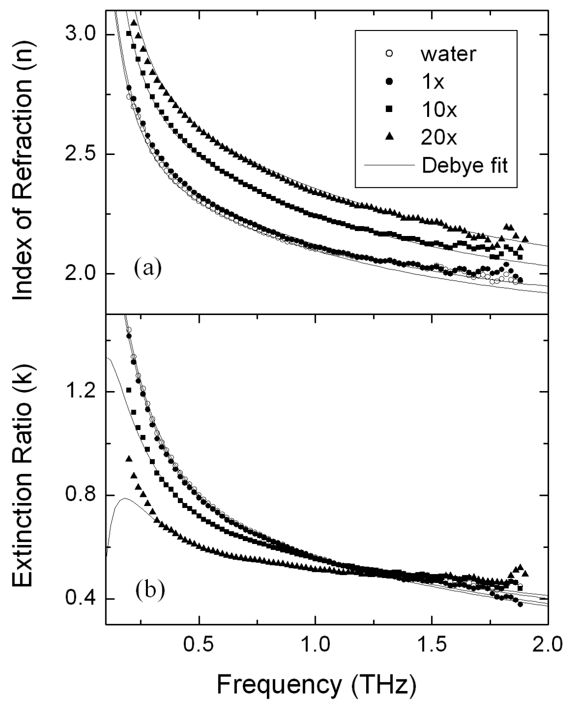

Fig. 1. (a) The refractive index and (b) the extinction ratio. The solid lines are the fit into the modified double Debye model.

The mixture in water has many motions in the terahertz region such as formation and breakage of the hydrogen bond, and dipole rotational and translational motions. We use the modified double Debye model composed of complex dielectric constants and the specific conductance to represent these motions. The complex permittivity of the model is given by :

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_2}{1 + i\omega\tau_1} + \frac{\varepsilon_2 - \varepsilon_\infty}{1 + i\omega\tau_2} + \frac{i\sigma_0}{\varepsilon_0\omega} \qquad (1)$$

The solid lines in Figs. 1 and 2 represent the model fitted into the experimental data. The fitting constants are shown in Table 1.

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TABLE I

Debye model fitting parameters (ε_S : the static dielectric constant, ε_2 : the intermediate permittivity, ε_∞ : the infinite dielectric constant, τ_1 and τ_2 : the slow and fast relaxation times, σ_0 : the specific conductance at quasi-static)

	ε_S	ε_2	ε_∞	τ_1 (ps)	τ_2 (fs)	σ_0
water	78.50	4.95	3.25	7.75	169	0
1×	77.00	5.00	3.30	7.20	157	0.04
10×	61.40	5.75	3.45	3.80	149	0.53
20×	47.90	6.25	3.75	2.65	144	0.74
electrolytes	33.07	8.20	4.10	1.15	141	1.40

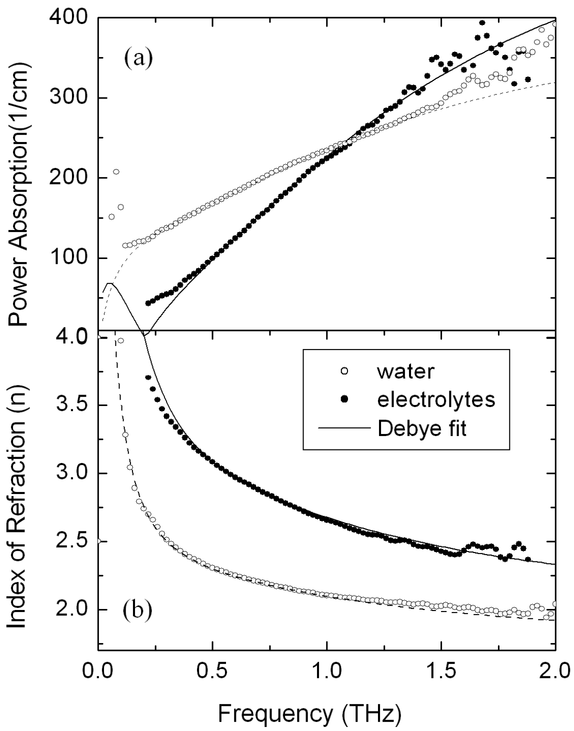

Fig. 2. (a) Power absorptions and (b) the refractive indices of the electrolytes in the LB medium (closed circle) and water (open circle) The solid lines represent the fit into the modified double Debye model.

As the concentration of ingredients increased, the slow reorientation time τ_1 and the fast reorientation time τ_2 were reduced from 7.75 to 2.65 ps and from 169 to 144 fs, respectively. The mixture's conductivity is almost proportional to the ingredients' concentration.

III. Disccusion

The mixture was deemed ideal by mass fraction to consist of two parts--water and electrolytes--to extract the properties of electrolytes only[2]. The power absorption α_{MIX} and the index of refraction n_{MIX} of the ideal mixture can be represented as follows :

$$\alpha_{MIX} = C_W \alpha_W + C_E \alpha_E \qquad (2)$$
$$n_{MIX} = C_W n_W + C_E n_E \qquad (3)$$

where α_W and α_E are the power absorptions of water and electrolytes, n_W and n_E are the indices of refraction of water and electrolytes, respectively, and C_W and C_E are the mass ratios of water and electrolytes to the total mixture, respectively. Power absorption and the refractive index of the electrolyte parts obtained for the sample are shown in Fig. 2. We have fitted the extracted values with the modified double Debye model. The slow and fast reorientation times of electrolytes decreased to 1.15 ps from 7.75 ps and to 141 from 169 of water, respectively. The specific conductance is increased to 1.4 from 0 of water. These results imply that the electrolytes in water do not need the hydrogen-bond breakage that take place in water under THz radiation.

IV. Conclusion

The biological mixture can be characterized in terms of optical constants such as complex indices of refraction, dielectric constants and conductivity. The ultrafast dynamics of the biological material, such as the hydrogen-bond breakage can be explained by the molecular dynamics model in terahertz region.

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