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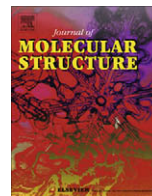


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Comparative dielectric study of pentanol isomers with terahertz time-domain spectroscopy

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ARTICLE INFO

Article history:

Received 17 January 2010

Received in revised form 28 February 2010

Accepted 1 March 2010

Available online 6 March 2010

Keywords:

Terahertz time-domain spectroscopy

Dielectric relaxation

Hydrogen-bonded liquids

Monohydric alcohols

Boson peak

Intermolecular vibration

ABSTRACT

Using terahertz (THz) time-domain spectroscopy, we have measured the complex permittivity of seven pentanol isomers (1-pentanol, 2-pentanol, 3-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 2-methyl-2-butanol, and 3-methyl-2-butanol) in the frequency range of 0.2–2.5 THz at temperatures from 253 to 323 K. For all samples, the complex permittivity contains the following three components: (i) a high-frequency side of dielectric relaxation processes, (ii) a broad vibration mode around 1.5 THz, and (iii) a low-frequency side of an intermolecular stretching mode located above 2.5 THz. At low temperatures, the relaxation process moves to a low-frequency range and a peak of the broad vibration mode, which is independent of temperature, is clearly observed around 1.5 THz. Spectra in the THz region change sensitively according to the molecular structure of the pentanol isomers. We have also observed the complex permittivity in the microwave range of 1 MHz–20 GHz. The behavior of the dielectric relaxation processes below GHz region much depend on the isomers. Our experimental data demonstrate that the molecular structures of the pentanol isomers influence all the molecular dynamics ranging from dielectric relaxation phenomena, which are due to reorientational motion of the molecules, to vibration dynamics within the hydrogen-bonded network structure.

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1. Introduction

“THz waves” is a generic term used to refer to electromagnetic waves of $0.1\text{--}10 \times 10^{12}$ Hz in frequency. Before efficient methods of THz wave emission and detection were established, the THz region was not studied extensively. However, emission and detection techniques for THz waves have been developed with a femtosecond laser and semiconductor device technology in recent years. THz waves are now attracting attention in fundamental and applied research. In the former, THz time-domain spectroscopy (THz-TDS) has been established [1,2], enabling us to accurately measure complex permittivity in the THz region.

The new experimental technique has proven to be a powerful tool for the study of molecular dynamics and interactions in various materials. The study of molecular dynamics in hydrogen-bonded liquids is one of the most important applications because of their significance in various fields such as physical chemistry, biology, and industry. In the THz region, molecular dynamics are expected to be related to the hydrogen-bonding phenomena that distinguish hydrogen-bonded liquids from simple liquids. Observa-

tion will therefore serve as a key to explaining complicated physical properties in hydrogen-bonded liquids.

In the present study, we have performed complex permittivity measurements of pentanol isomers (1-pentanol, 2-pentanol, 3-pentanol, 2-methyl-1-butanol, 3-methyl-1-butanol, 2-methyl-2-butanol, and 3-methyl-2-butanol) with THz-TDS. These structural isomers differ in the position of the OH group and the structure of the carbon chain, which affects the formation of hydrogen bonds in the liquid state. The objective of this study is to perform systematic experiments with pentanol isomers in the THz region. On basis of the experimental results, we will discuss the underlying microscopic mechanisms contributing to dielectric spectra in this frequency range.

2. Experimental

The experimental technique of THz-TDS has been well developed and described in detail by others [3–5]. A mode-locked Ti sapphire laser (Tsunami, Spectra Physics), which generates femtosecond pulses with the wavelength of 800 nm, was used for the emission and detection of pulsed THz waves. For the emission, we produced a photoconductive antenna with electrodes, the gap distance of which is 500 μm , fabricated on a semi-insulating

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gallium arsenide substrate. In the detection of THz pulses, an electro-optic (EO) sampling method was employed with a <1 1 0> ZnTe crystal (1 mm in thickness) as an EO crystal. The wave path was enclosed in a vacuum box (below 20 Pa) to reduce absorption by atmospheric water vapor.

Liquid samples were put into the sample cell consisting of a pair of polypropylene windows and a spacer. The temperature of liquid sample was controlled from 253 to 323 K by a Peltier device. (Except for 2-methyl-2-butanol, whose melting point is 261 K, measurements for this sample were made from 263 to 323 K.) The sample thickness was controlled by the spacer (500 and 1000 μm). The THz pulses transmitted through an empty cell were first recorded followed by collection of data for the liquid samples. The complex permittivities of pentanol isomers were calculated with the Fourier transforms of the THz waves transmitted through the samples and the empty sample cell. Typical experimental errors in both dielectric permittivity and dielectric loss were 5% for the whole frequency range.

Data in the microwave range were also obtained to study dielectric properties of pentanol isomers in a wide frequency range. For the measurement of the microwave range, two different experimental setups were used in order to cover the frequency ranges between 1 MHz and 20 GHz. From 1 to 500 MHz, the complex permittivity measurements were performed with a network analyzer (HP4195A). From 500 MHz to 20 GHz, the complex permittivity was obtained by time domain reflectometry [6–8]. Concerning the experimental details in the microwave region, we refer the reader to our previous paper [9]. The temperature of the sample in both experimental setups was controlled at 273–323 K.

The molecular structures of pentanol isomers used in this study are indicated in Fig. 1. 1-Pentanol was purchased from Kanto Chemical, 3-methyl-1-butanol was purchased from Kishida Chemical, 3-methyl-2-butanol was purchased from Junsei Chemical, and other alcohols were purchased from Wako Pure Chemical Industries. All these chemicals were of analytical grade (97.0–98.5%) and were used without further purification. In the case of 2-methyl-1-butanol and 3-methyl-2-butanol, the chemicals obtained were a mixture of the optical isomers.

3. Results and discussion

3.1. Complex permittivity in the THz region

Fig. 2(a)–(g) show the complex permittivities $\varepsilon^*(\omega) = \varepsilon'(\omega) - i\varepsilon''(\omega)$ of all the pentanol isomers studied. Some dielectric relaxa-

tion processes below the GHz frequency region in monohydric alcohols have been reported [10–14]. These processes contribute to $\varepsilon'(\omega)$ in the THz region, resulting in the rise in dielectric permittivity $\varepsilon'(\omega)$ and dielectric loss $\varepsilon''(\omega)$ below 0.5 THz in Fig. 2(a)–(g). With decreasing temperature, these relaxation processes shift to a lower frequency range, leading to the decrease in dielectric loss values below 0.5 THz. After this shift, a peak can be clearly seen around 1.5 THz; the peak position is almost independent of temperature. Furthermore, above 2.0 THz, a rise in the dielectric loss is observed for almost all pentanol isomers, which indicates the location of another mode above 2.5 THz. To sum up the basic characteristics of the complex permittivities of pentanol isomers in the THz region, they contain three contributions: (i) a high-frequency side of dielectric relaxation processes, (ii) a mode with peak position around 1.5 THz, and (iii) a low-frequency side of another mode located above 2.5 THz. We will examine these contributions more closely in the following sections.

3.2. Peak in the dielectric loss around 1.5 THz

Let us begin our discussion by considering a peak observed in the dielectric loss $\varepsilon''(\omega)$ around 1.5 THz. In the present study, by lowering the temperature down to 253 K, the mode with peak position around 1.5 THz is clearly observed in pentanol isomers. This mode shows a broad vibration feature as demonstrated in Fig. 3 with the fitting results of two functions: Debye function [Eq. (1)] and Lorentz function [Eq. (2)]. The Debye function [15] is used to represent the simplest dielectric relaxation process which has one relaxation time. On the other hand, the Lorentz function has been introduced to fit the vibration mode of hydrogen-bonded liquids in the THz region [14,16,17].

$$\varepsilon^*(\omega) = \frac{\Delta\varepsilon}{1 + i\omega\tau} \quad (1)$$

$$\varepsilon^*(\omega) = \frac{A}{\omega_0^2 - \omega^2 + i\omega\gamma_0} \quad (2)$$

In Fig. 3, the Lorentz function can represent the mode around 1.5 THz, which indicates that the mode arises from vibration dynamics, while the Debye function cannot express the narrow shape of the mode.

Studies on molecular dynamics of hydrogen-bonded liquids in the THz region have been conducted with other experimental and theoretical techniques. In water and lower alcohols, which are representatives of hydrogen-bonded liquids, some vibration dynamics were reported to be observed in the THz region. Previous

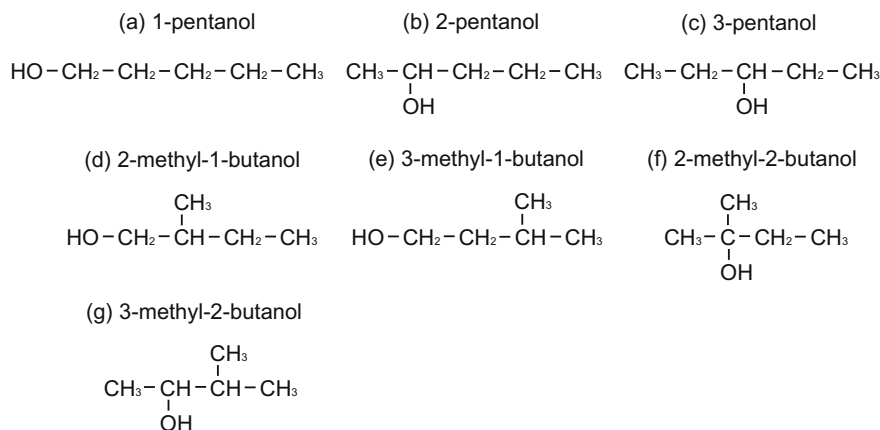


Fig. 1. Molecular structure of (a) 1-pentanol, (b) 2-pentanol, (c) 3-pentanol, (d) 2-methyl-1-butanol, (e) 3-methyl-1-butanol, (f) 2-methyl-2-butanol, and (g) 3-methyl-2-butanol.

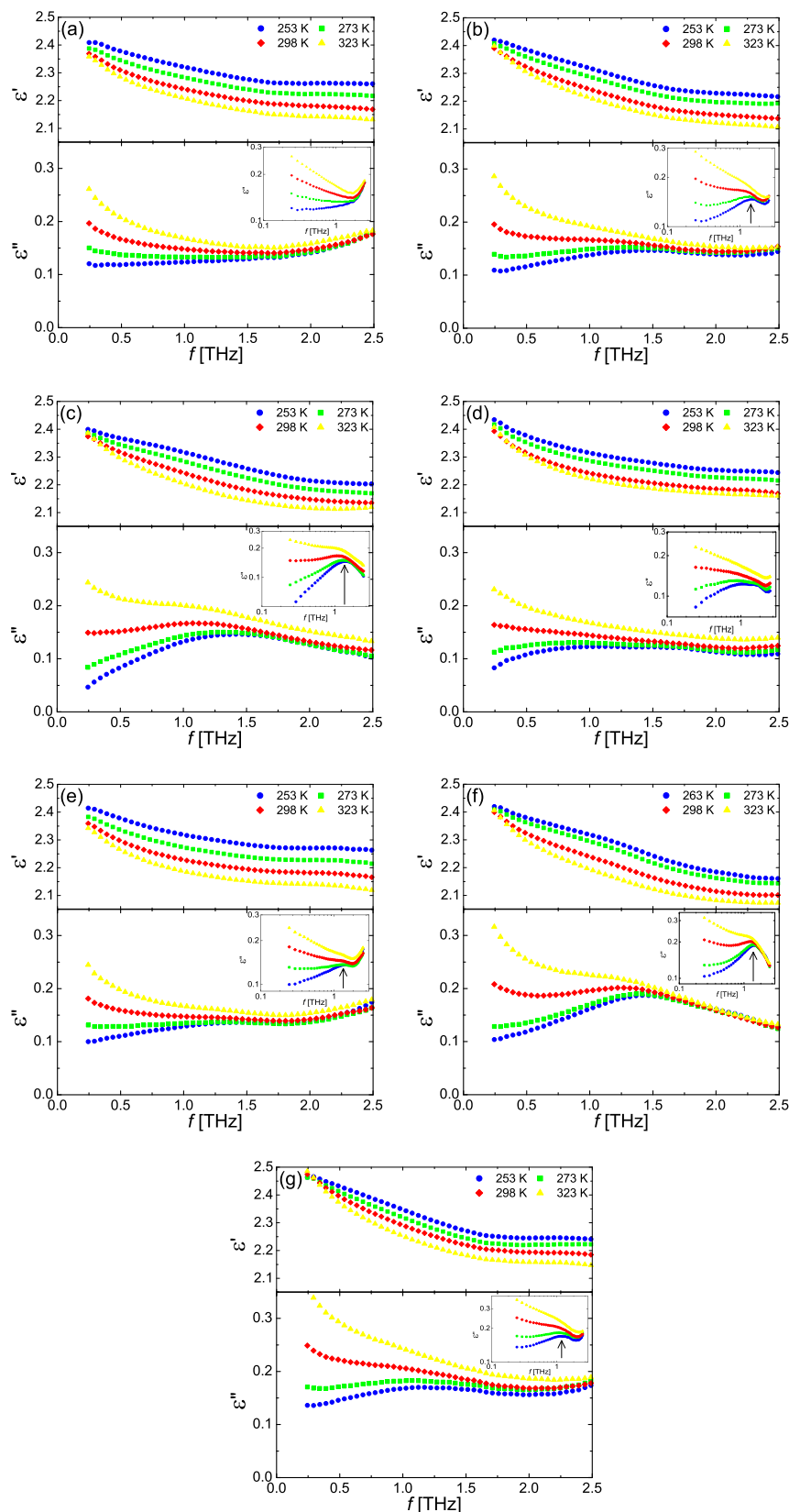


Fig. 2. Dielectric permittivity (upper panel) and dielectric loss (lower panel) of (a) 1-pentanol, (b) 2-pentanol, (c) 3-pentanol, (d) 2-methyl-1-butanol, (e) 3-methyl-1-butanol, (f) 2-methyl-2-butanol, and (g) 3-methyl-2-butanol in the frequency range between 0.2 THz and 2.5 THz at 253–323 K. Inset in lower panel shows bilogarithmic plot of dielectric loss.

Raman scattering studies [18,19] of water observed intermolecular vibrations such as hydrogen-bond bending at $\sim 50 \text{ cm}^{-1}$ and hydrogen-bond stretching at $\sim 180 \text{ cm}^{-1}$. As for methanol, some

theoretical and experimental studies [20–23] reported several intermolecular vibrations and the fluctuation of the methyl group below 100 cm^{-1} . These vibration dynamics can be candidates for

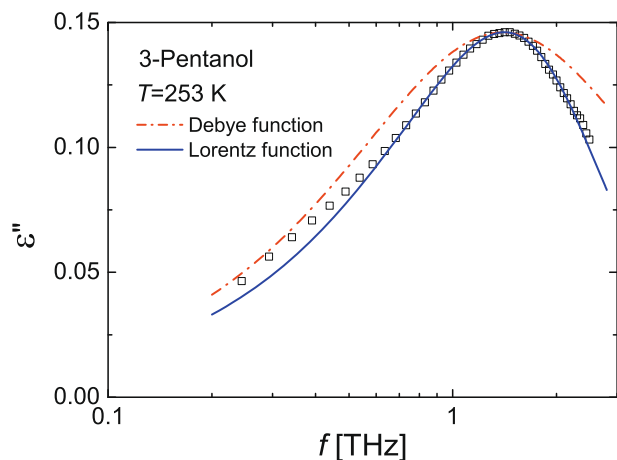


Fig. 3. Dielectric loss of 3-pentanol at 253 K. Open rectangles represent our experimental data. Dashed-dotted curve and solid curve represent fitting by Eqs. (1) and (2), respectively.

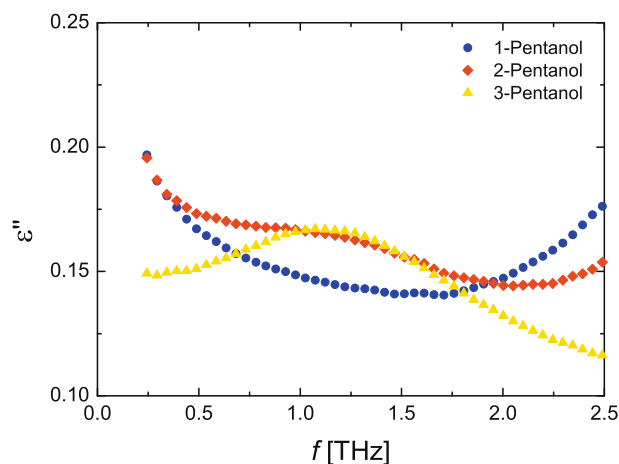


Fig. 4. Comparison of dielectric losses of 1-pentanol, 2-pentanol, and 3-pentanol.

the origin of the mode around 1.5 THz in pentanol isomers. Other molecular dynamics can also be expected to exist due to the larger molecular structure of the pentanol isomers compared with water and methanol. However, in the present state of knowledge, the origin of the mode around 1.5 THz cannot possibly be decided. Woods et al. [22,23] reported about water–methanol mixtures wherein they found that addition of small amounts of water lead to the deformation of the methanol network structure, which changed the appearance of the absorption bands below 100 cm^{-1} . This result indicated that the low-frequency vibration dynamics is sensitive to the local structure in hydrogen-bonded liquids.

The appearances of the vibration mode around 1.5 THz differs in shape and intensity according to the molecular structures [Fig. 2(a)–(g)]. First, we focus on the position of the OH group in a molecule. The position of the OH group in 1-pentanol is at the terminal carbon atom, whereas the OH group in 2-pentanol and 3-pentanol is at the middle position of the carbon chain. Fig. 4 shows that the intensities of the vibration mode of 2-pentanol and 3-pentanol are higher than that of 1-pentanol. Fig. 5 compares the dielectric losses of 2-methyl-1-butanol, 2-methyl-2-butanol, 3-methyl-1-butanol and 3-methyl-2-butanol. In addition, the isomers that have the OH group at the middle position of the carbon chain (2-methyl-2-butanol and 3-methyl-2-butanol) show higher intensity of the mode than isomers with the OH group at the terminal carbon atom (2-methyl-1-butanol and 3-methyl-1-butanol).

Second, let us examine the influence of the carbon chain structure on the mode around 1.5 THz in Figs. 6 and 7. 1-Pentanol, 2-methyl-1-butanol, and 3-methyl-1-butanol have an OH group at a terminal carbon atom, while the structures of the carbon chain differ. In this

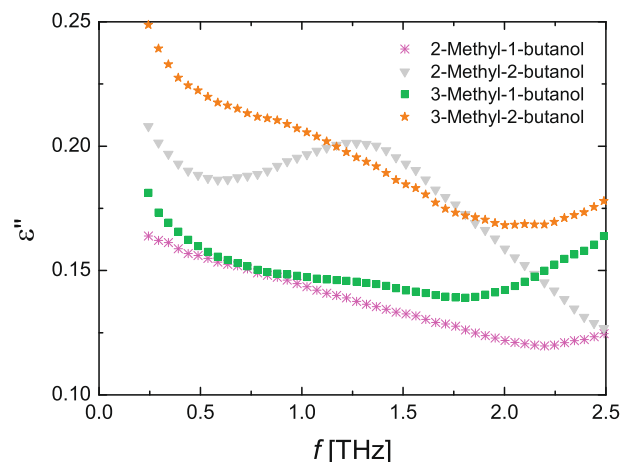


Fig. 5. Comparison of dielectric losses of 2-methyl-1-butanol, 2-methyl-2-butanol, 3-methyl-1-butanol, and 3-methyl-2-butanol.

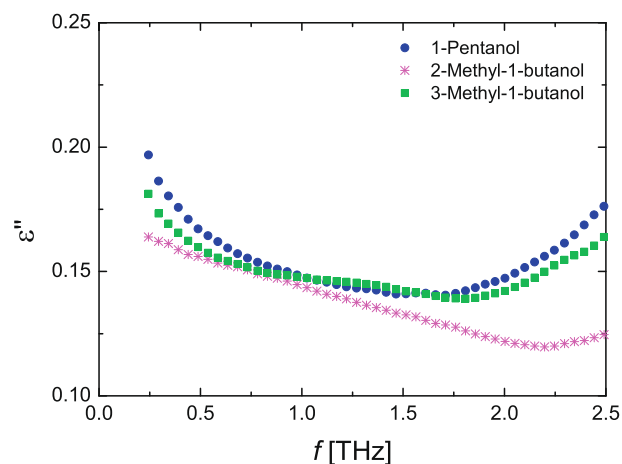


Fig. 6. Comparison of dielectric losses of 1-pentanol, 2-methyl-1-butanol, and 3-methyl-1-butanol.

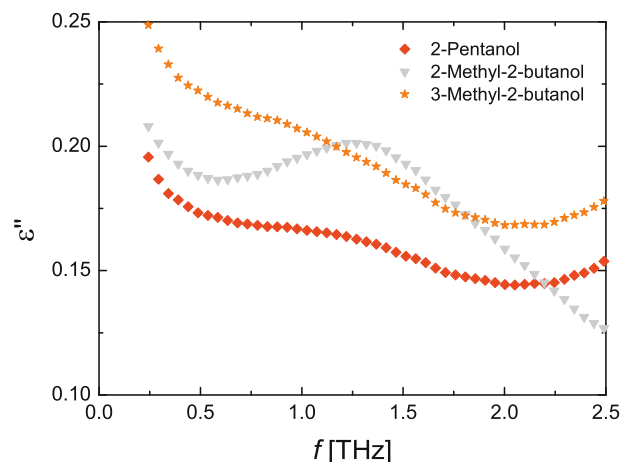


Fig. 7. Comparison of dielectric losses of 2-pentanol, 2-methyl-2-butanol, and 3-methyl-2-butanol.

series of pentanol isomers (Fig. 6), the appearance of the vibration mode around 1.5 THz are similar. On the other hand, in the comparison between 2-pentanol, 2-methyl-2-butanol, and 3-methyl-2-butanol, which have an OH group at the middle position of the carbon chain, the intensity of the mode changes according to the chain structure (Fig. 7). In this case, the difference in the carbon chain structure affects the vibration mode. As has been observed, the vibration mode around 1.5 THz is influenced by both the position of the OH group and the carbon chain structure.

The peak positions of the dielectric loss around 1.5 THz are given in Table 1. The values of the peak position were estimated from data at 253 K to possibly exclude the contribution of the high-frequency tail of dielectric relaxation processes. (Except for 2-methyl-2-butanol, whose melting point is 261 K, the peak position was estimated at 263 K.) Although we cannot exclude the contribution completely, the peak positions change depending on the molecular structure. The peak positions are distinguishable in almost all isomers, as indicated by arrows in the insets of Fig. 2(a)–(g). However, for 1-pentanol and 2-methyl-1-butanol, the peaks are very broad, and it is difficult to distinguish the peak positions, unlike the other isomers. Future investigations are necessary to pinpoint the cause of the difference in spectral shape; we will not examine this difference in detail here.

Another important discussion is about the relationship of the vibration mode around 1.5 THz with the boson peak which is generally observed in the supercooled liquid state and in the glass state. The experimental frequency range which can be covered by THz-TDS corresponds to the range where the boson peak is generally observed. The boson peak in monohydric alcohols has been investigated with several experimental techniques. Yamamuro et al. [24,25] performed the neutron scattering measurement of 1-propanol in the glass state and showed that a boson peak was identified at 2–3 meV in the dynamical structure factor. This energy level almost corresponds to the frequency range where the vibration mode around 1.5 THz is observed in our study. Yamamuro et al. concluded that the origin of the boson peak in alcohols is related to alkyl groups which are flexible side chains in the hydrogen-bonded network. Since the temperature range in our study was limited, we could not attain the glass state of pentanol isomers. Future investigations at much lower temperatures are necessary for the discussion of the boson peak. From such experiments, the boson peak will be analyzed in detail and the relationship of the boson peak in the glass state and the vibration mode in the THz region will be clarified.

3.3. Rise in the dielectric loss above 2.0 THz

Previous studies of low-frequency Raman scattering and infrared absorption spectroscopy [26–28] have shown that an intermolecular stretching mode exists above 2.0 THz in monohydric alcohols. For example in 1-pentanol, the intermolecular stretching mode was observed at 150 cm^{-1} [26]. From this result, it is reasonable to suppose that the rise in dielectric loss above 2.0 THz in pentanol isomers is caused by the low-frequency side of this intermolecular stretching mode. In this study, we cannot observe the whole picture of the intermolecular vibration mode. Therefore, it

is difficult to discuss it in detail with only our data. However, the rise in the dielectric loss toward 2.5 THz clearly shows that the intermolecular stretching mode, as well as the vibration mode around 1.5 THz, is strongly influenced by the molecular structures of pentanol isomers. Further expansion of the experimental frequency range above 2.5 THz will clarify the relationship of the molecular structure with the intermolecular stretching mode.

3.4. Dielectric relaxation processes below GHz range

We also measured the complex permittivity in the microwave region. As examples of measurements in a wide frequency range, Fig. 8(a)–(c) present the complex permittivities of 1-, 2-, and 3-pentanol, respectively, in the range of 1 MHz–2.5 THz. In the present study, the dominant dielectric relaxation process in the pentanol isomers is represented by the Debye function [15], as shown in Fig. 8(a)–(c). The temperature dependence of relaxation frequency f_m of the dominant process is expressed by Eq. (3) for pentanol isomers in our temperature range.

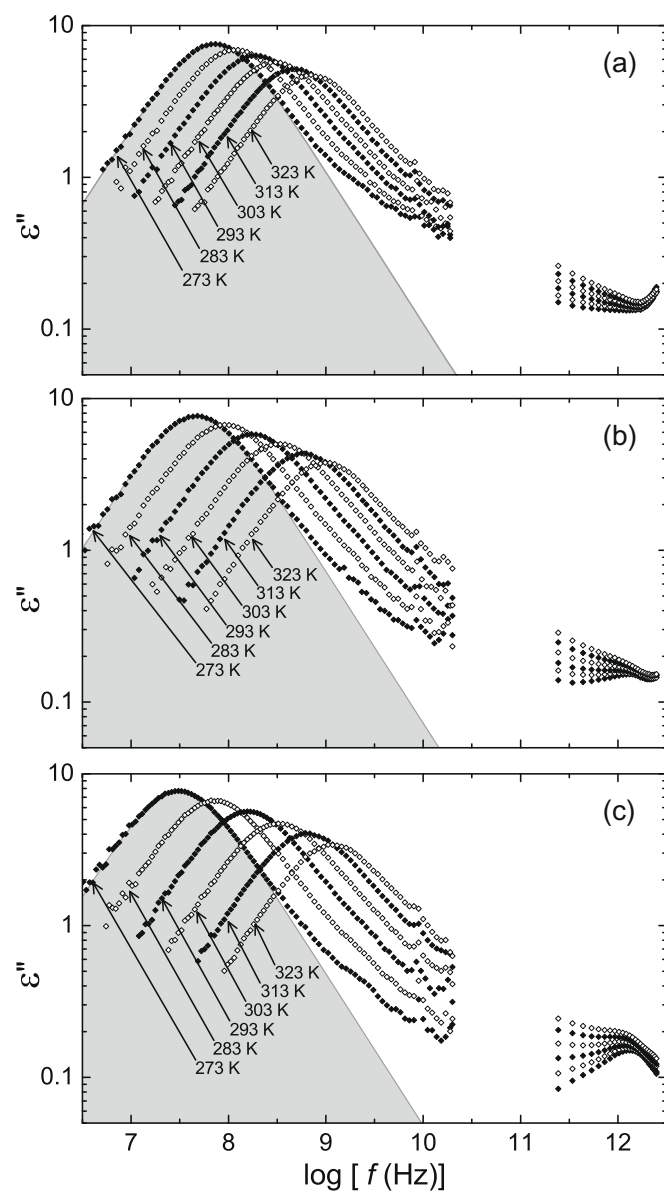


Fig. 8. Dielectric loss of (a) 1-pentanol, (b) 2-pentanol, and (c) 3-pentanol in the frequency range between 1 MHz and 2.5 THz at 273–323 K. Gray-shaded area represents fitting by the Debye function for 273 K.

Table 1
Peak positions of the dielectric loss in the THz region.

	Peak position [THz]
2-Pentanol	1.43
3-Pentanol	1.47
2-Methyl-2-butanol	1.44
3-Methyl-1-butanol	1.47
3-Methyl-2-butanol	1.17

Table 2

Calculated activation energies of the dominant Debye-type dielectric relaxation process.

	Activation energy [kJ/mol]
1-Pentanol	33.4
2-Pentanol	44.6
3-Pentanol	53.7
2-Methyl-1-butanol	41.3
3-Methyl-1-butanol	35.4

$$\log f_m = \log f_0 - \frac{\Delta E}{2.303RT} \quad (3)$$

Here, R is the gas constant, T is the absolute temperature, ΔE is the activation energy associated with the dipole orientation, and f_0 represents the extrapolated frequency at $T \rightarrow \infty$. The activation energies of some pentanol isomers are determined by Eq. (3), and the values are listed in Table 1. The temperature dependence of the dominant process depends greatly on the isomers, although the molecular structures of these isomers differ only slightly from each other. Thus, the activation energy of the dominant process changes with the isomer (Table 2). Shinomiya [29] reported the dielectric study of 1-, 2-, and 3-pentanol in the range of 1.35 MHz–4.5 GHz at 15, 25, and 35 °C. In the study, the dominant dielectric relaxation process was described by the Debye function, the same as our estimation. The activation energies of the process were 30.9 for 1-pentanol, 41.9 for 2-pentanol, and 49.5 kJ/mol for 3-pentanol, respectively. Although the values in our study are large, about 7% difference compared with theirs, they have the same tendency; the activation energy increases as the OH group approaches the center of a molecule. Shinomiya interpreted the increase as the shielding effect of the carbon chain for an OH group, which restricts the hydrogen-bonding rearrangement. In the present study, we also investigated 2-methyl-1-butanol and 3-methyl-1-butanol to check the influence of the carbon chain structure on the activation energy. The activation energy of 3-methyl-1-butanol is smaller than that of 2-methyl-1-butanol. This result indicates that the branch position of the carbon chain near the OH group has larger steric hindrance effect on the rearrangement. Generally, the dominant Debye-type process in monohydric alcohols is ascribed to cooperative dynamics of molecules in the hydrogen-bonded network [10–14]. Cooperative relaxation dynamics is strongly influenced by the change in the carbon chain structure and the position of the OH group of pentanol isomers.

Furthermore, in the high-frequency side of the dominant process, the deviation from the Debye-type process is seen in the dielectric loss [Fig. 8(a)–(c)]. It has been reported that the deviation can be expressed by the combination of two Debye-type dielectric relaxation processes in monohydric alcohols [10–14]. For these alcohols, despite their simple molecular structures, three dielectric relaxation processes coexist in a wide frequency range. This is clearly because these alcohols form a hydrogen-bonded network through intermolecular hydrogen bonds. Although two high-frequency dielectric relaxation processes are not fully assessed in our study due to the limited frequency range, it is clear that the high-frequency processes change dramatically according to the isomers [Fig. 8(a)–(c)].

Thus, our experimental data have demonstrated that the molecular structures of pentanol isomers influence all the molecular dynamics ranging from dielectric relaxation phenomena, which are due to reorientational motions of molecules, to intermolecular vibration dynamics within the hydrogen-bonded network structure.

4. Conclusions

We have measured the complex permittivity of seven pentanol isomers with THz-TDS. The molecular structures of these isomers change systematically with the position of the OH group and the structure of the carbon chain. The complex permittivities studied contain three contributions: (i) a high-frequency side of dielectric relaxation processes, (ii) a vibration mode around 1.5 THz, and (iii) a low-frequency side of an intermolecular stretching mode located above 2.5 THz. The dielectric spectra in the THz region change sensitively according to the molecular structures of the pentanol isomers. We also measured the complex permittivity in the microwave range. The dominant Debye-type process is also influenced by the molecular structure. Our experimental data indicate that the molecular structures of the pentanol isomers influence all the molecular dynamics ranging from reorientational motion of the molecules to vibration dynamics within the hydrogen-bonded network structure.

At the moment, we can fully discuss contribution (ii) (a broad mode around 1.5 THz). However, the discussion of contributions (i) (high-frequency side of dielectric relaxation processes) and (iii) (low-frequency side of an intermolecular vibration mode located above 2.5 THz) cannot be further expanded due to the limited frequency range. A further direction of our work will be to extend the experimental frequency range. To discuss all the contributions in the THz region, it is necessary to fill the gap between 20 GHz and 0.2 THz and expand the frequency range above 2.5 THz. Addition of these “missing” frequency ranges to the current results will aid the understanding of the entire molecular dynamics within the hydrogen-bonded network in monohydric alcohols. The present study is important as the starting point of such an attempt.

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