

Assignment of terahertz vibrational mode in sucrose powder by comparing with single-crystalline and computational spectra

T. Ohashi¹, K. Takahashi², H. Sato² and H. Takaba³

¹ Production Engineering Center, IHI Corporation, Yokohama, 235-8501 JAPAN

² Research Laboratory, IHI Corporation, Yokohama, 235-8501 JAPAN

³ Department of Environmental and Energy Chemistry, Kogakuin University, Hachioji, 192-0015 JAPAN

Abstract— It is necessary to get assignment of spectra originated with specific vibrational mode of organic compounds for the practical or industrial application of terahertz spectroscopy. Terahertz spectra of single crystal and powdered sucrose were measured and compared with computational spectrum. The result shows good agreement, and represents the possibility to assign the origin of peaks in the terahertz spectra.

I. INTRODUCTION

In the terahertz band, it can be observed intermolecular and intramolecular vibrational mode related with hydrogen bonding or Van-der-Waals force. Therefore terahertz spectroscopy is expected to be helpful tool for understanding such weak interactions between organic molecules.

For the practical or industrial application of terahertz spectroscopy, it is necessary to get assignment of spectra originated with specific vibrational mode. In this study, terahertz spectra of single crystal and powdered sucrose were measured, respectively. Moreover, measured spectra were compared with computational spectrum calculated by density functional theory (DFT) method to assign the spectral peaks with their vibrational mode.

II. MATERIALS AND METHODS

Single crystals of sucrose (shown in Fig. 1) were used through all measurement, and powdered sucrose was prepared by mortar pulverization from the single crystals.

Fig. 2 shows three different crystal planes of sucrose; a-axis face cut (A-cut), c-axis face cut (C-cut) and ab-axis face cut (AB-cut). A-cut contains vibration modes originated from b- and c- axes. On the other hand, C-cut plane contains that originated from a- and b- axes.



Fig. 1. Single crystal of sucrose.

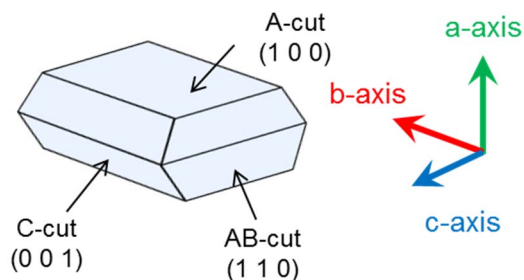


Fig. 2. Three different crystal planes of sucrose single crystal.

All terahertz spectra were collected by high resolution terahertz time-domain spectrometer (TH-01, IHI Corporation), and measured under varying temperature. The spectra obtained at 80 K were adopted to compare with computational spectra.

Computational spectra were calculated using the density functional method using a plane wave basis function. The initial crystal structure for the calculation was obtained X-ray diffraction measurement at 143 K.

III. RESULTS

Terahertz spectra of single crystal were measured in different crystal plane. As a result, specific spectra related in each crystal axis were observed. Fig. 3 depicts axis-dependent terahertz spectra observed by rotating the A-cut sample. Fig. 3 (a) shows the spectrum obtained by terahertz wave of parallel polarization with the b-axis of A-cut plane, while Fig. 3 (b) shows that obtained by the wave of parallel polarization with c-axis of A-cut plane. Those spectra clearly show the difference originated from the direction of the molecular vibrations.

Correspondingly, similar results were obtained from C-cut sample shown in Fig. 4. Fig. 4 (a) shows the spectrum obtained by terahertz wave of parallel polarization with the a-axis of C-cut plane, while Fig. 4 (b) shows that obtained by the wave of parallel polarization with b-axis of C-cut plane. Moreover, b-axis spectra, obtained from A-cut and C-cut, were nearly identical. Thus, we were able to gain an effective result to assign the spectrum terahertz vibrational mode of sucrose single crystal.

Comparisons of experimental and computational spectra are depicted in Fig. 5. The spectra of single crystal sucrose were calculated by averaging a-, b, and c-axis spectra. Fig. 5 (a) and (b) show the spectra obtained by powdered and single crystal sucrose. Obviously, they have good relationship in their spectra, suggesting powdered sucrose consist of small single crystal.

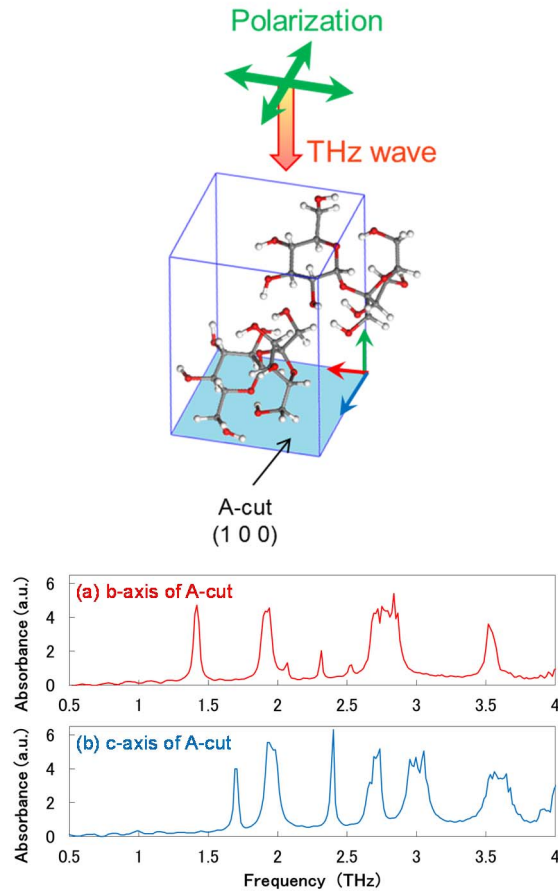


Fig. 3. The axis-dependent spectra of A-cut sucrose single crystal between 0.5–4.0 THz at 80 K. Spectra were measured of (a) b-axis of A-cut sample (red), (c) c-axis of A-cut sample (blue).

Furthermore, computational spectrum, shown in Fig. 5 (c), also represents good agreement with both powdered and single crystal sucrose experimental spectra. Hence, these results represent the possibility to assign the origin of peaks in terahertz spectra.

IV. SUMMARY

In this study, terahertz spectra of single crystal and powdered sucrose were measured, respectively. Moreover, measured spectra were compared with computational spectrum calculated by DFT method to assign the spectral peaks with their vibrational mode.

Terahertz spectra of single crystal were measured in different crystal plane, and specific spectra related in each crystal axis were observed. The result clearly shows the difference originated from the direction of the molecular vibrations. Thus, we were able to gain an effective result to assign the spectrum terahertz vibrational mode of sucrose single crystal.

Both experimental spectra, obtained by powdered and single crystal sucrose, obviously showed good relationship in their spectra, suggesting powdered sucrose consists of small single crystal. Furthermore, comparison of experimental and computational spectrum also represents good agreement. Hence, these results represent the possibility to assign the origin of peaks in terahertz spectra.

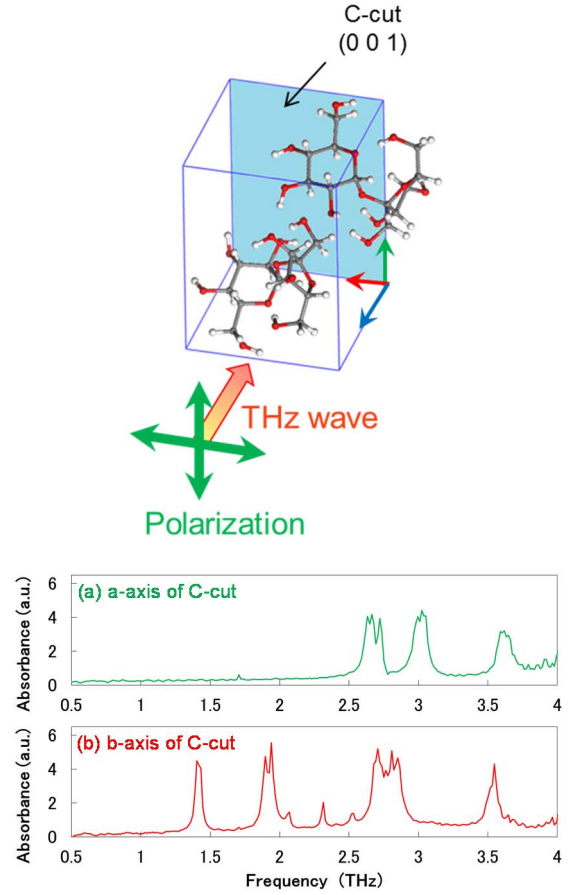


Fig. 4. The axis-dependent spectra of C-cut sucrose single crystal between 0.5–4.0 THz at 80 K. Spectra were measured of (a) a-axis of C-cut sample (green), (b) b-axis of C-cut sample (red).

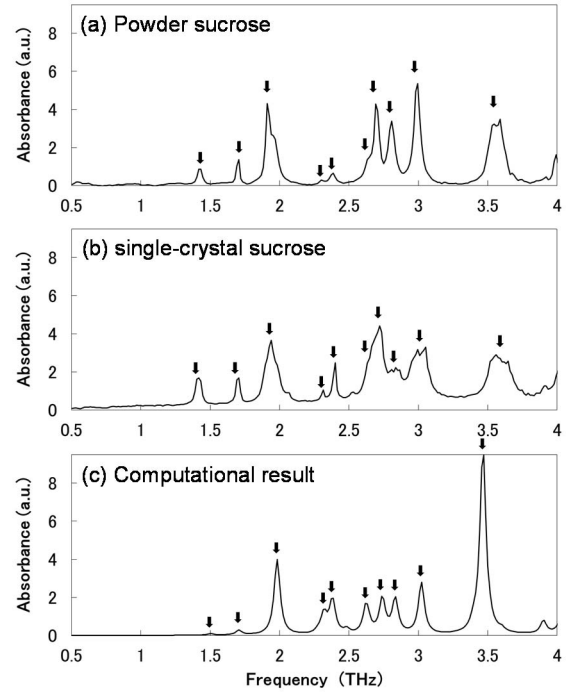


Fig. 5. Comparison of THz spectra of (a) powder sucrose, (b) single crystal sucrose and (c) computational result.