Special polarization characteristic features of a three-dimensional terahertz photonic crystal semi-quantitatively evaluated by using a FEM

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Abstract

A previous work [1] experimentally confirmed that the special polarization characteristic features of a three-dimensional terahertz (THz) photonic-crystal with a silicon inverse diamond structure whose lattice point shape was vacant regular octahedrons, did not apparently apply to general physical and optical basic rules. One of the basic rules is that, according to Maxwell’s equations, the electric-field direction of the reflected wave rotates by 180 degrees from that of the incident wave in the case of complete reflection (Bragg reflection) and normal incidence. It is said that three-dimensional photonic crystals have no polarization anisotropy within photonic band gap (stop gap, stop band) of high symmetry points in normal incidence. Experimental results, however, confirmed that the polarization orientation of a reflected wave was different from that of an incident wave. In this work, measured reflected spectra in the previous work were semi-quantitatively evaluated by being compared with reflection ones by using a FEM (finite element method). These results suggest that measured polarization anisotropy does not apply to Maxwell’s equations in appearance but applies to these equations in essential as expected.

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Introduction

The previous work, ref. [1] with the polarization anisotropy, which was the polarization orientation difference between the reflected wave and the incident one, confirmed that new reflection phenomena of a three-dimensional (3D) terahertz photonic-crystal (PC) with a silicon inverse diamond structure whose lattice point shape was vacant regular octahedrons, did not apparently apply to general physical- and optical-basic rules.

These basic rules are as follows.

(A) Electric-field ($E$) is vector, and various optical phenomena are analyzed by using methods of resolution and synthesis of $E$.

(B) According to Maxwell’s equations that are electromagnetic basic rules, $E$-direction (polarization orientation) of the reflected wave rotates by 180 degrees from that of the incident wave in the case of complete reflection (Bragg reflection) and normal incidence.

(C) According to crystallography, diamond structure is in cubic system and optically isotropic.

Polarization features in ref. [3] do not also apply to rule (B) except complete reflection and rule (C). The features exist in frequencies without photonic band gap (PBG). The 3D-PC has eigen modes (branches) in these frequencies. Each eigen mode has an intrinsic symmetry, and some polarization anisotropy also exists.

In ref. [4], the direction- and wavelength-dependent polarization anisotropy of stop gap branching has been studied with fcc symmetry as a function of an incidence angle for two polarization orientation normal to each other, TE and TM.

In the previous work, however, the polarization anisotropy in normal incidence and within X point’s PBG, BGX in fig. A.1 (appendix), was entirely different from above characteristics; no eigen modes based on the 3D-band structure exist within BGX. None the less because some two directions at right angles to each other on the plane (001) are constitutionally and optically identical, the polarization orientation of the reflected wave rotated by 90 degrees from that of the incident wave at a frequency, 0.42 THz within BGX when that of the incident wave was the direction that bisects these two directions.

The general outline of ref. [1] is shown in fig. 1. The comparison of the polarization characteristic features as generally expected in fig. (a) with ones in the measured spectra in fig. (c) is shown. I(X,Y) in fig. (b) is the polarization orientation of the incident wave. The unit cell of a diamond structure in fig. 2 is illustrated. The incident wave is normal incidence, [001] (Γ-X direction). The solid arrow is the polarization orientation of the incident wave, and the dashed arrow is that of the reflected wave. The frequency of the incident wave is 0.42 THz within BGX.

General characteristic features of the polarization indicate that the polarization orientation of the reflected wave is parallel to that of the incident wave as shown in fig. (a). The features of the polarization

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1 Ref. [1] contains more detailed analyses than those in ref. [2].

2 [001] and (001) are defined on the X-Y-Z coordinate system in fig. 2.
in the measured spectra, however, indicated entirely different ones as shown in fig. 1(c); the polarization orientation of the reflected wave was perpendicular to that of the incident wave when that of the incident wave was $[I(±1, 0)]$ or $[I(0, ±1)]$.

In contrast, when that of the incident wave is $[I(±1, ±1)]$ or $[I(±1, ±1)]$ (double sign in same order), no polarization anisotropy existed experimentally. In other words, the polarization orientation of the reflected wave was parallel to that of the incident wave. According to rule (A), when that of the incident wave is $[I(±1, 0)]$ or $[I(0, ±1)]$, the polarization orientation of the reflected wave is parallel to that of the incident wave. The experimental facts, however, indicated that the former was perpendicular to the latter. These facts do not apparently apply to rule (A), in addition, the characteristic features do not apply to the general theory of the 1/2 wave plate in appearance.

In this work, reflected and transmission spectra of the 3D-PC were analyzed by using a FEM (finite element method), and these simulation spectra were semi-quantitatively made comparisons with the measured spectra.

**Parameters**

The FEM software was Femtet(R)2017.1 made in Murata Software Co., Ltd.. The model size in this work was from 1500 $\mu$m to 1800 $\mu$m on a side. Several models were analyzed with the size magnified a hundred times since the maximum drawing size was 1000 $\mu$m and 1000 mm when analysis unit was $\mu$m and mm, respectively. The scaling rule is applicable in the photonic crystals. In other words, frequency $\times$ size (lattice constant) is constant. On the base of this rule, the spectrum frequencies were finally shifted from GHz to $0.1 \times$ THz as the size needed to be reduced by a hundredth. The following explanations use final sizes ($\mu$m) and final frequencies (THz).

In addition, the software had no command to obtain S-polarization (S-p) spectra and P-polarization (P-p) ones separately. Only compound spectra of S-p and P-p were able to be obtained.

The unit cell of the simulation model is the diamond structure as shown in fig. 2(a). The sphere is the lattice point and its shape is the regular octahedrons in fig. 2(b). It is vacant (atmosphere) and the dielectric constant, $\varepsilon_1 = 1.00$ was set. The surrounding material is pure Si and the dielectric constant, $\varepsilon_2 = 11.9$ was set.

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3In this theory, the two directions orthogonal each other are optically anisotropic.

4S-p and P-p are orthogonal each other. Two polarization are explained in detail in fig. A.2.
The lattice constant, \( a = 300 \mu m \) and the side length of the regular octahedrons, \( L = 150 \mu m \) were set in the theoretical and experimental works. In the unit cell of the Si inverse diamond structure, many sections of the air octahedrons on the lattice points are arranged as shown in figs. 2(c) and 2(d).

Fig. A.1(a) shows the calculated photonic band structure by using plane wave expansion method. In this work, the direction of the incident wave was +Z-direction, [001] in the real space and it corresponds to \( \Gamma-X \) direction on the \( K_z \)-axis in the wave number space (K-space). The polarization anisotropy was studied on the surface (001) at around BGX.

The relationship between reflectivity \( R(\text{XY}) \), transmittance \( T(\text{XY}) \) and the polarization orientations of the incident wave, \( I(\text{XY}) \) is explained as follows. Four orientations of \( I(0, \pm 1) \) and \( I(\pm 1, 0) \) are constitutionally and optically comparable as shown in fig. 2(b). They are totally expressed as \( I(10) \). For the same reason, four orientations, \( I(\pm 1, \pm 1) \) are also totally expressed as \( I(11) \). The reflectivity, \( R \) is expressed as \( R(10) \) or \( R(11) \) when the incident wave is \( I(10) \) or \( I(11) \), respectively, and the transmittance, \( T \) is similarly expressed as \( T(10) \) or \( T(11) \) when the incident wave is \( I(10) \) or \( I(11) \), respectively.

Furthermore, both \( R(10) \) and \( R(11) \) are compound spectra of S-p and P-p of the reflected wave. \( T(10) \) and \( T(11) \) are also the same in meaning.

In more detail, firstly, (10) and (11) correspond to the polarization orientation of the incident wave, secondly, S-p of the reflected wave means the polarization component parallel to the polarization orientation of the incident wave, thirdly, P-p of the reflected wave means the polarization component perpendicular to S-p.

Two analyzed models are model(11) and model(10) as shown in fig. 3. X-Y-Z coordinate system corresponds to that in fig. 2. The model size is \( L_a \times L_a \times L_b \) (\( \mu m \))^3. \( L_b \) is the height of the Z-direction. \( L_a \times L_a \) is the area in X-Y plane. The square area surrounded with white dashed lines is \( a \times a \) (\( \mu m \))^2, which corresponds to that in fig. 2(d). port is shown as the square surrounded with black heavy lines. It is the area of the incident wave, whose size is \( L_p \times L_p \) (\( \mu m \))^2. The white heavy arrow is the orientation of the electric-field vector, \( E_1 \) of the incident wave, which is

\[ R(f) = RS(f) + RP(f) \]

\[ T(f) = TS(f) + TP(f) \]

The variable, \( f \) is a THz frequency. \( RS \) (TS) is S-p reflectivity (transmittance). \( R(10) \) is \( R(10)(f) \), exactly.
Fig. 3: Two analyzed models are model(11) and model(10). The square surrounded with black heavy lines, port is the area of the incident wave. The white heavy arrows are the orientation of the electric-field vector of the incident wave.

The direction of the incident wave is +Z-direction and normal incidence. The location correlation between I(XY) and model(XY) is as follows.

- **model(11)**: \( E_I \parallel (Y = -X) \); I(11)
- **model(10)**: \( E_I \parallel X \); I(10)

Table 1: Five kinds of model size. \( R_e \) is reflectivity and \( T_r \) is transmittance.

| (\( R_e, T_r \))          | 3D-PC size                  | port size        |
|--------------------------|-----------------------------|------------------|
| \( (R_{11}, T_{11}) \)   | \((L_a \times L_a \times L_b)\) | \((L_p \times L_p)\) |
| \( (R_{10}, T_{10}) \)   | \((5a \times 5a \times 5a)\) | \((4a \times 4a)\) |
| \( (R_{10}, T_{10}) \)   | \((6a \times 6a \times 5a)\) | \((3a \times 3a)\) |
| \( (R_{10}, T_{10}) \)   | \((6a \times 6a \times 5a)\) | \((3a \times 3a)\) |
| \( (R_{10}, T_{10}) \)   | \((6a \times 6a \times 5a)\) | \((4a \times 4a)\) |
| \( (R_{10}, T_{10}) \)   | \((6a \times 6a \times 5a)\) | \((5a \times 5a)\) |

Table 1: Five kinds of model size. \( R_e \) is reflectivity and \( T_r \) is transmittance.

PBG’s in fig. 4 are nearly equal to BGX in fig. A. The reflectivity is large and transmittance is very small within PBG. In model(11) [figs. 4(a), 4(c) and 4(e)], the shapes of three reflected spectra are approximately convex downward within PBG, which is similar characteristic to one another. In model(10) [figs. 4(b), 4(d) and 4(f)], the shapes of the reflected spectra display concavity and convexity within PBG. The shapes of the spectra depend on the 3D-PC size and port size since these size are small.

In the case of the same port size, for instance, \( (R_i, T_i) \) (i = B and C), the spectra are similar each other in model(10). \( R_D \) was also similar spectra to \( R_A \). As the port size is larger, reflectivity within PBG

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6 The model size is nearly maximum for the limit of the personal computer's performance: OS: Windows 10 Home (64bit), processor: Intel(R) Core (TM) i5-6500 CPU@3.20 GHz, RAM: 64.0 GHz.

7 Four S-parameters were calculated in the FEM software. They are \( S_{11} \), \( S_{22} \), \( S_{21} \), and \( S_{12} \). Reflectivity and transmittance correspond to \( |S_{11}|^2 \) and \( |S_{21}|^2 \), respectively.
is larger. Two local maximum values of $R_E(10)$ are 0.82 and 0.93 as shown in fig. 5. It is thought that as the port size becomes large, the ratio of a scattering wave to the reflected wave becomes small and then the reflectivity becomes large. The shapes of the reflected spectra in PBG also change to a certain degree.

In the sub-peaks of reflected spectra and transmission ones without PBG in figs. 4(a) to 4(f), local maximum value and local minimum one of two spectra tend to appear at the same frequency as expected.

**Experimental results**

The measured reflected spectra, and the reflected ones obtained from them, in ref. [1], are shown in fig. 6. The total number of layered chips of the sample was 28. The height of one chip is 75 µm, and the height of the sample corresponds to $7a$. The reflection and transmission measurement systems are shown in fig. A.2. Fig. 6(a) shows $RP(11)$ (white circle), $RS(11)$ (cross shape) and $R(11)$ (black circle). $R(11) = RP(11) + RS(11)$. The polarization orientation of the incident wave is I(11), which corresponds to the white heavy arrow in fig. A.2(b). 90°-spectrum (white circle) in fig. A.2(a) corresponds to $RS(11)$, and 90°-spectrum in fig. A.2(b) corresponds to $RP(11)$. $RP(11)$ is very small, and $R(11)$ is nearly equal to $RS(11)$. 
Fig. 6: $R(11)$ and $R(10)$ are compound reflected spectra. $RS(11)$ and $RS(10)$ are measured $S$-p reflected spectra. $RP(11)$ and $RP(10)$ are measured $P$-p ones. $R(11) = RP(11) + RS(11)$. $R(10) = RP(10) + RS(10)$.

Fig. 6(b) shows $RP(10)$ (white circle), $RS(10)$ (cross shape) and $R(10)$ (black circle). $R(10) = RP(10) + RS(10)$. The polarization orientation of the incident wave is I(10), which corresponds to the white heavy arrow in fig. 3(d). $45^\circ$-spectra (black circle) in figs. A4(a) and A4(b) correspond to $RS(10)$ and $RP(10)$, respectively. At 0.42THz, $RS(10)$ is very small, and $R(10)$ is nearly equal to $RP(10)$.

Fig. 7 shows $R(11)$, $T(11)$, $R(10)$ and $T(10)$. $T(11) = TS(11) + TP(11)$. $T(10) = TS(10) + TP(10)$. $T(11)$ and $T(10)$ are nearly equal to zero within BGX.

The number of side peaks without BGX depends on the layered number that corresponds to the height of $Z$-direction. The height of the total layered chips, $7a$ is larger than $5a$ that is the height of the simulation model. The number of side peaks in the measured spectra is larger than those in the simulation ones.

Discussions

Fig. 8 shows $R_E(11)$ and $R_E(10)$, whose model sizes are shown in table 1, and $R(11)$ and $R(10)$ in fig. 7. The frequency range of $R(11)$ and $R(10)$ is indicated within 0.338THz to 0.464 THz. These values deviate from BGX slightly owing to process and fabrication accuracy and so on.

The spot size’s diameter of the incident wave in the measurement is about $20a$ (6mm)\(^8\), which is much larger than the port size, $5a \times 5a$ in table 1. The scattering ratio to the measured reflected wave is able to be nearly neglected. Therefore, in BGX, the measured reflectivity is probably larger than the simulated one.

In fig. 8(a), $R_E(11)$ and $R(11)$ are approximately convex downward and similar spectra within BGX. Meanwhile, in fig. 8(b), $R_E(10)$ and $R(10)$ display concavity and convexity within PBG, which are characteristics in common. Within BGX, $R_E(11)$ and $R(11)$ have smoother concavo-

\(^8\)The sample size is $33a \times 33a \times 7a$ in ref. [1].
Fig. 8: The comparison of simulation reflected spectra (black circle) with measured ones (white circle).

convex shape than $R_{E}(10)$ and $R(10)$ do, relatively.

Conclusions

The results of above discussions suggest that the polarization anisotropy of the measured reflected spectra do not apply to Maxwell’s equations in appearance but apply to these equations in essential as expected.

References

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Appendix

Some figures shown in ref. [1] and transmission measurement system in this work are collectively indicated in the appendix.

Fig. A. 1: (a) The calculated photonic band structure has complete photonic band gap, CPB (gray zone) at around 0.4 THz. BGX exists from 0.36 THz to 0.44 THz. (b) The first Brillouin zone and the reduced zone (heavy line) with high symmetry points.
Fig. A. 2: The conceptual diagram of the measurement system with a THz-TDS. (a) reflection measurement system. (b) transmission measurement system. The polarization orientation of a THz wave from the emitter is S-p x-axis and the detector detects only S-p. Another polarization perpendicular to S-p is P-polarization (P-p) that is included in the incidence plane // z-axis. The designed 1/2 wave plate converts S-p into P-p and P-p into S-p at around 0.42 THz. This plate was used only in the case of P-p detection. S(±P) means S-p, P-p or the mixing of S-p and P-p. In fig. A.2(a), the 3D-PC sample is so horizontally set that the layered direction is parallel to Z-axis. It is parallel to Z-axis in fig. 2. In this work, the 3D-PC sample was rotated in plane (001) instead of the S-p incident wave, relatively. The incident angle, φ is 7°, which is the normal incidence approximately.

Fig. A. 3: The transmittance, WS(f) of the designed 1/2 wave plate at around 0.42 THz. For instance, S-p incident wave is nearly converted into P-p at 0.42 THz. The dash line includes the signal disposal from the back surface of the 1/2 wave plate. The solid line includes no disposal.

Fig. A. 4: The measured reflected spectra, RS(f), RP(f), RS(f) × WS(f) and RW(f) from 0.2 THz to 0.6 THz for θ = 0° to 90° per 15°. The vertical solid line is 0.42 THz-line. RS(f) is the S-p reflectivity with no 1/2 wave plate in fig. A.2(a), whose polarization orientation is parallel to that of the incident wave. RS(f) is normalized by the Au reflection spectra. RW(f) is the normalized reflectivity passing through the 1/2 wave plate. RP(f) is the P-p reflectivity that is defined as [RW(f) − RS(f) × WS(f)]/[1 − WS(f)].