Choice of optimal crystal-orientation for terahertz transceiver with zincblende crystal*

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This paper presents a set of equations describing the terahertz generation and electro–optic detection based on optical rectification in zincblende crystals. The dependence of terahertz emission efficiency on the polarization of incident beam and crystal-orientation is discussed. For the experimental setup with a transceiver which transmits and detects terahertz radiation in the same crystal, we have demonstrated the optimal combination of both parameters above to optimize the working efficiency. Equations supplied in this paper are valid for zincblende crystals with arbitrary crystal-orientation and every possible polarization of an incident beam, which are of great significance for the optimization of a system.

Keywords: terahertz transceiver, optical rectification, electro–optic detection, optimal orientation

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1. Introduction

The generation and detection of free space terahertz (THz) radiation have been extensively investigated in the last two decades. Many works have been done to obtain efficient and compact THz devices such as emitters and detectors.[1−6] The THz radiation sources based on the optical rectification in the semiconductor[7−11] under the ultrafast laser pulse excitation and the THz electro–optic (EO) sampling detection[12−15] have attracted more attention since they are convenient to be employed with desirable performance.

The THz generation by optical rectification is a second-order nonlinear optical process. In addition, the EO detection is basically regarded as a reverse process of its rectified generation, thus it is more convenient to realize detection and generation on one crystal as a transceiver.[16] Because the THz generation and detection processes are accomplished in one crystal in a transceiver, which decrease the flexibility of the system, the transceiver has a limited signal-to-noise ratio. However, the transceiver has a smaller size than a traditional THz generation and detection system, which makes it desirable for cases where a portable and compact THz system is needed. It is well known that THz generation and detection based on optical rectification can be strongly affected by the crystallographic orientation, the azimuthal angle of EO crystals and the polarization of incident beam.[17−20] When realizing the generation and detection on one crystal, these effects become more complex and make it very difficult to determine the optimum transceiver conditions. Chen *et al.* made significant investigations of the crystal-orientation-dependent efficiency of an EO THz transceiver constructed by (110) and (111) zincblende crystals.[20] In the paper of Nick *et al.* some expressions describing the EO detection were given for general propagation directions of the probe beam and the THz field.[21] However, there are no detailed descriptions and expressions for the general situation of an EO crystal with an arbitrary crystal orientation and an incident beam with an arbitrary polarization direction, which are obviously important to THz generation and detection.

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This paper gives a full mathematic description of THz emission and EO detection based on the second-order nonlinear optical effect in zincblende crystal. We show the dependence of the generation and detection of the THz field on the crystal-orientation and the polarization of the incident beam. Since orientation and polarization are chosen arbitrarily, our results are valid in general cases. It should be noted that there are three coordinate systems utilized in our calculation, all the relevant vectors expressed in different coordinate systems can be distinguished by their superscripts.

2. Calculation

2.1. Terahertz wave generation in zincblende crystals

When the optical pump beam with an ultrafast pulse train irradiates on an EO nonlinear crystal, the different frequency components interact and form a beating polarization, which radiates electromagnetic waves at the beat frequency.[22] The amplitude of the radiated electric field is proportional to the second-order time derivative of the dielectric polarization in the far-field approximation. In this section, we give a detailed theoretical description of the crystal-orientation-dependent generation of THz radiation.

As shown in Fig. 1, we define a laboratory coordinate system xyz with the x axis as the crystal-orientation and perpendicular to the crystal surface, the incident plane is the x–z plane. In addition, we express the crystallographic coordinate system as $x'y'z'$ with $[1,0,0] \to x'$, $[0,1,0] \to y'$ and $[0,0,1] \to z'$. The third coordinate system is defined as follows: the x'' axis coincides with the x axis and satisfies the transformation

$$\begin{aligned}
\hat{\boldsymbol{x}}'' &= s_{x'}\hat{\boldsymbol{x}}' + s_{y'}\hat{\boldsymbol{y}}' + s_{z'}\hat{\boldsymbol{z}}',\\
\hat{\boldsymbol{y}}'' &= (-s_{z'}\hat{\boldsymbol{y}}' + s_{y'}\hat{\boldsymbol{z}}')\Big/\sqrt{s_{y'}^2 + s_{z'}^2},\\
\hat{\boldsymbol{z}}'' &= \big[(s_{y'}^2 + s_{z'}^2)\hat{\boldsymbol{x}}' - s_{x'}s_{y'}\hat{\boldsymbol{y}}'\\
&\quad - s_{x'}s_{z'}\hat{\boldsymbol{z}}'\big]\Big/\sqrt{s_{y'}^2 + s_{z'}^2}, \qquad (1)
\end{aligned}$$

where $\hat{x}'$, $\hat{y}'$, $\hat{z}'$ are the unit vectors of the crystallographic coordinate system, $\hat{x}''$, $\hat{y}''$, $\hat{z}''$ are the unit vectors of the third coordinate system, $s_{x'}$, $s_{y'}$, $s_{z'}$ are the components of the unit vector $\hat{x}''$ respect to crystallographic axes. For an EO crystal with a zincblende structure, the nonlinear susceptibility is expressed in the crystallographic coordinate system as[23]

$$d_{ijk} = d_{il} = \begin{bmatrix} 0 & 0 & 0 & d_{14} & 0 & 0\\ 0 & 0 & 0 & 0 & d_{14} & 0\\ 0 & 0 & 0 & 0 & 0 & d_{14} \end{bmatrix}. \qquad (2)$$

Under the situation of normal incidence, the incident optical beam can be written as

$$E_{\text{pump}} = (0, E_y, E_z) = E_0(0, \sin\varphi, \cos\varphi), \qquad (3)$$

where E_z, E_y are amplitudes of z (p-polarization) and y (s-polarization) component of incident beam, respectively.

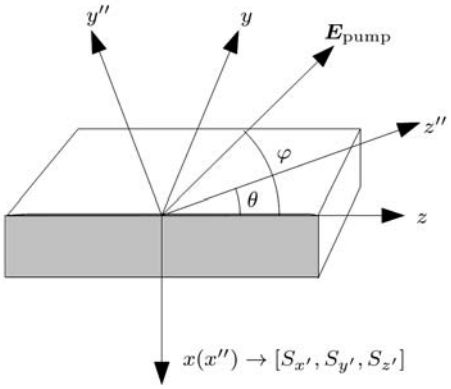


Fig. 1. Geometry of the crystal and coordinate systems. The surface of the crystal is y–z plane, the x–z plane is defined as the incident plane. The x'' axis coincides with the x axis whose direction is $[s_{x'}, s_{y'}, s_{z'}]$ expressed in an $x'y'z'$ coordinate system. The azimuth θ is defined as the angle between the z axis and the z'' axis. The $\boldsymbol{E}_{\text{pump}}$ is the electric field vector of the incident beam (normally incident), which has an angle φ with z axis.

After some calculations and transformations, we obtain the expression of nonlinear polarization P''[24]

$$P'' = \begin{bmatrix} P_{x''}\\ P_{y''}\\ P_{z''} \end{bmatrix} = \frac{8E_0^2 d_{14}}{(n_{\text{pump}}+1)^2} \begin{bmatrix} \dfrac{\sqrt{1-C}}{C}\left(\dfrac{A(2C-1)}{2(1-C)}\sin 2(\varphi-\theta) + \dfrac{B}{2}((2-3C)\cos 2(\varphi-\theta) - 3C)\right)\\ -\dfrac{1}{\sqrt{C}}\left(\dfrac{A}{2}\cos 2(\varphi-\theta) + B\sin 2(\varphi-\theta) + \dfrac{A}{2}\right)\\ \dfrac{1}{2\sqrt{C}}\left(B((4-3C)\cos 2(\varphi-\theta) + 2 - 3C) - 2A\sin 2(\varphi-\theta)\right) \end{bmatrix}, \qquad (4)$$

where $n_{\rm pump}$ is the refractive index of the incident beam in the crystal and

$$A = s_{x'}(s_{y'}^2 - s_{z'}^2), \quad B = s_{y'}s_{z'}, \quad C = s_{y'}^2 + s_{z'}^2. \tag{5}$$

Because the amplitude of the radiated THz electric field is proportional to the nonlinear polarization and the THz electric field in the x'' direction cannot be coupled out from the crystal,[16] so the expression of the radiated THz electric field is

$$\begin{bmatrix} E_{{\rm THz}y''} \\ E_{{\rm THz}z''} \end{bmatrix} \propto \frac{8E_0^2 d_{14} n_{\rm THz}}{(n_{\rm pump}+1)^2(n_{\rm THz}+1)} \frac{2}{\sqrt{C}} \begin{bmatrix} -\left(A\cos^2(\varphi-\theta) + B\sin 2(\varphi-\theta)\right) \\ B((4-3C)\cos^2(\varphi-\theta)-1) - A\sin 2(\varphi-\theta) \end{bmatrix}, \tag{6}$$

where $E_{{\rm THz}y''}$, $E_{{\rm THz}z''}$ are the components of the THz electric field $E_{\rm THz}$ in the y'', z'' directions, respectively, $n_{\rm THz}$ is the refractive index of the THz wave in the crystal. In Eqs. (4) and (6), we have considered the transmitted coefficients of amplitude when a polarized beam crosses the interface of crystal.

Note that in Eq. (6), the THz electric field is affected by the angle $\varphi - \theta$, which indicates the relative position of polarization of the incident beam and the azimuth of the crystal. So it is convenient for experimenters to just fix the polarization direction φ or azimuth θ, and modify the other to vary the magnitude of the THz field. Assume that the crystal orientation is set to be $\hat{S} = [s_{x'}, s_{y'}, s_{z'}] = [\cos\alpha\sin\beta, \sin\alpha\sin\beta, \cos\beta]$, where α, β are polar angles of vector $\hat{S}$ in the crystallographic coordinate system. The maximum absolute values of the THz electric field ($|E_{\rm THz}| = (|E_{{\rm THz}y''}|^2 + |E_{{\rm THz}z''}|^2)^{1/2}$) can be achieved with different orientation $\hat{S}$, which are plotted in Fig. 2(a). The THz field reaches a maximum when the values of (α, β) are set to $(0, \pi/2)$, $(\pi/2, \pi)$, and $(\pi, \pi/2)$, all of which correspond to $\langle 110\rangle$ orientation. The THz field gradually diminishes from $\langle 110\rangle$ orientation to $\langle 100\rangle$ and $\langle 111\rangle$ orientation, and vanishes at $\langle 100\rangle$ orientation which agrees well with the published results. Furthermore, we found that there are same maximums of the THz field at some other orientations, all optimum crystal-orientations are shown in Fig. 2(b). However, it is reasonable to use crystal with $\langle 110\rangle$ orientation because it is a sophisticated commercial product. As seen from Fig. 2(a), the THz field changes slowly near the optimal orientations. So a small deviation from the optimal orientations can exert a very limited influence on the generation of THz radiation.

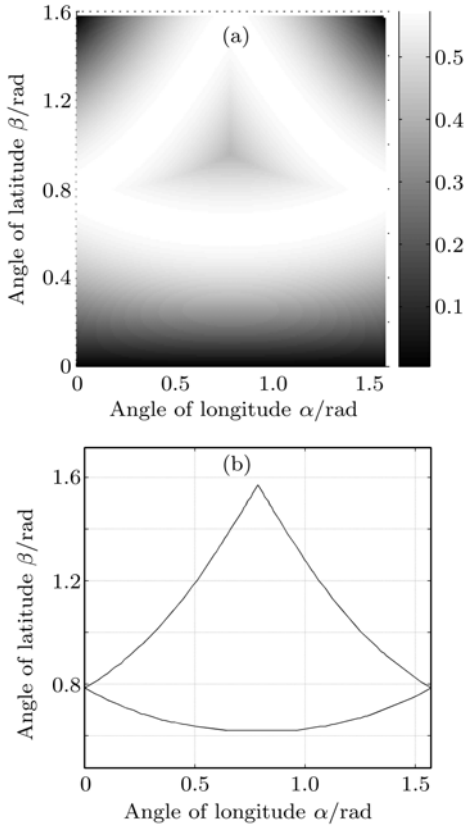


Fig. 2. (a) The maximums which can be obtained for the THz electric field as a function of crystal-orientation expressed by longitude α and latitude β. (b) Optimum crystal-orientations for maximizing the THz field.

2.2. Terahertz detection by EO sampling

When an arbitrary bias electric field is applied to the EO crystal, the electric field will induce a refractive-index change which affects the ellipticity of the index ellipsoid. This change in ellipticity is measured by comparing the two orthogonal polarization components of the probe beam separated by a polarizing beam splitter. A balanced photodetector measures the intensity difference between the two components and gives a signal that is directly proportional to the applied electric field. A typical EO detection setup is displayed in Fig. 3.

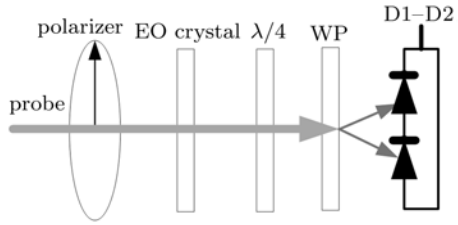


Fig. 3. Schematic diagram of the general experimental setup of EO detection. A probe beam, which is linearly polarized after passing a polarizer, travels through an EO crystal and $\lambda/4$ plate, and is then split by a Wollaston prism (WP). A differential detector (consisting of photodiodes D1 and D2) measures the difference D1–D2, which is proportional to the THz electric field applied to the EO crystal.

When an arbitrary bias electric field $E' = (E_{x'}, E_{y'}, E_{z'})$ is applied to an EO crystal with a zincblende structure, the equation of the crystal refractive-index ellipsoid can be expressed as[25]

$$\frac{x'^2 + y'^2 + z'^2}{n_0^2} + 2r_{41}E_{x'}y'z' + 2r_{41}E_{y'}z'x' + 2r_{41}E_{z'}x'y' = 1 \qquad (7)$$

in the crystallographic coordinate system $\hat{x}'$, $\hat{y}'$, $\hat{z}'$. In most cases, the probe illuminates the surface of the crystal vertically, so we should rewrite Eq. (7) in the laboratory coordinate system $\hat{x}$, $\hat{y}$, $\hat{z}$ and set $x = 0$ to obtain the equation of the refractive-index ellipse of y–z plane. From the equation, we derive the two semiaxes n_1, n_2 and corresponding polarization directions $\hat{r}_{c1}$, $\hat{r}_{c2}$ of two propagation mode.[26] As shown in Fig. 4, we illustrate the polarization change of the probe beam passing the optical elements.

The polarization can be decomposed along directions $\hat{r}_{w1}$, $\hat{r}_{w2}$, respectively, when the probe beam passes the WP and splits into two beams, which are received by the two photodiodes, D1 and D2, respectively. We use I_1 and I_2 to express the intensities incident on the two photodiodes, the difference of the two intensities is given by Ref. [21]

$$\begin{aligned}\Delta I &= I_1 - I_2 \\ &\simeq I_0[\cos(2(\delta+\varphi))\cos(2(\gamma-\delta)) \\ &\quad + \phi\sin(2(\xi+\varphi))\sin(2(\gamma-\delta))], \end{aligned} \qquad (8)$$

where $I_0 = \varepsilon_0 c\sqrt{\varepsilon_r}\,|E_{\text{probe}}|^2/2$, $\phi = \omega L\Delta n/c$ is the phase difference of two propagation modes after the EO crystal, $\Delta n = n_1 - n_2$ is the refractive-index difference, ω, L, c are radian frequency of probe beam, the thickness of EO crystal and the velocity of light in vacuum, respectively. When there is no THz electric field applied to the EO crystal, $\phi = 0$ and the two intensities should be balanced to suppress the background noise, so it must be $\cos(2(\delta+\varphi)) = 0$ or $\cos(2(\gamma-\delta)) = 0$. Because $\delta+\varphi$ depends on the polarizations of probe beam, which is variable. So it is more reasonable to orientate the WP relative to the quarter-wave plate to make $\cos(2(\gamma-\delta)) = 0$. So the signal we obtained by the EO detection is expressed as

$$\Delta I/I_0 \simeq \sin(2(\xi+\varphi))\frac{\omega L\Delta n}{c}. \qquad (9)$$

From Eq. (9) we found that the signal is linear with the refractive–index difference induced by THz field applied to the EO crystal. The $\xi+\varphi$ is the angle between the polarization of probe and the polarization of the propagation modes in the EO crystal. Both $\xi+\varphi$ and Δn depend on the applied THz electric field.

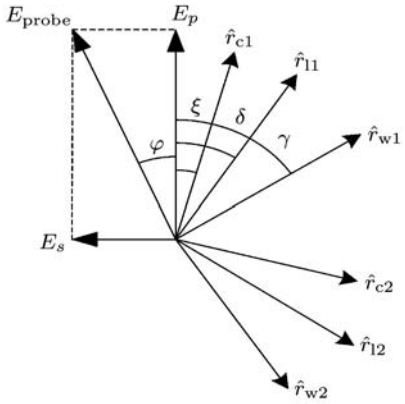


Fig. 4. The polarization directions of the two propagation modes in optical elements. The $\hat{r}_{c1}, \hat{r}_{c2}$ and $\hat{r}_{l1}, \hat{r}_{l2}$ are the polarizations direction of the two propagation modes in the EO crystal and $\lambda/4$ plate separately, the polarization directions of the two modes after WP are $\hat{r}_{w1}$, $\hat{r}_{w2}$. The E_p, E_s are p- and s-polarization components of the incident probe beam. The angle between E_p and $\hat{r}_{c1}$ is ξ, the angle between E_p and $\hat{r}_{l1}$ is δ, and the angle between E_p and $\hat{r}_{w1}$ is γ. All vectors are in the plane of paper and parallel to the surface of crystal because the probe beam and the THz wave applied to crystal propagate collinearly and perpendicularly to the crystal surface.

If we write the initial polarization of the probe beam in the coordinate system $x''y''z''$ as

$$\hat{E}''_{\text{probe}} = (0, \cos\eta, \sin\eta), \qquad (10)$$

where we use η to express the angle between the initial polarization direction of probe and the $\hat{y}''$ vector. So Eq. (9) can be rewritten as[21]

$$\begin{aligned}\Delta I/I_0 &\simeq \frac{\omega L n_0^3 r_{41}}{c}(E'_{\text{THz}} \cdot (S'_1\sin 2\eta + S'_2\cos 2\eta)) \\ &= \frac{\omega L n_0^3 r_{41}}{c}(E'_{\text{THz}} \cdot V') \end{aligned} \qquad (11)$$

with

$$S_1' = \left(s_{y'} s_{z'} \frac{s_{z'}^2 + s_{y'}^2 - 2}{s_{z'}^2 + s_{y'}^2}, s_{x'} s_{z'}, s_{x'} s_{y'} \right), \quad (12)$$

$$S_2' = \left(s_{x'} \frac{-s_{z'}^2 + s_{y'}^2}{s_{z'}^2 + s_{y'}^2}, -s_{y'}, s_{z'} \right), \quad (13)$$

$$V' = S_1' \sin 2\eta + S_2' \cos 2\eta. \quad (14)$$

All vectors in these equations are expressed in the coordinate system of crystallographic axes. It should be noted that equation. (11) is valid in any coordinate system, we can re-express it in the coordinate system $x''y''z''$ to simplify the calculation. By the selection of η, both the size and direction of V'' can be manipulated. For obtaining the maximum of the inner product of E''_{THz} and V'', we need only calculate the maximum of the $V''_{\parallel}$, which is the component of V'' parallel to the $y''z''$ plane. The signal $\Delta I/I_0$ can be expressed as follows:

$$\frac{\Delta I}{I_0} \simeq \left| V''_{\parallel} \right| = \left[\frac{(A\sin(2\eta) + 2B\cos(2\eta))^2 + (B(3C-4)\sin(2\eta) + 2A\cos(2\eta))^2}{C} \right]^{1/2}. \quad (15)$$

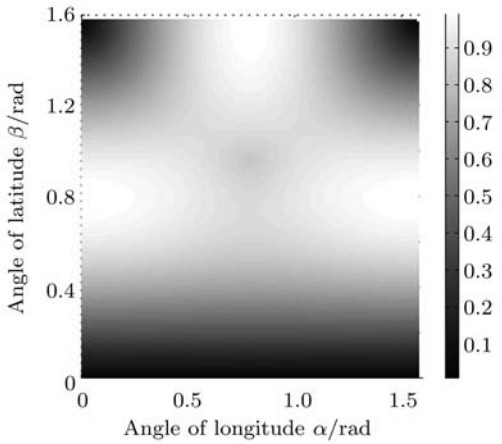


Fig. 5. The signal (arbitrary units) of EO detection with a separate EO crystal as a function of crystal-orientation expressed by longitude α and latitude β.

As shown in Fig. 5, we plot the maximum signal value (arbitrary units) as a function of the crystal-orientation of the EO crystal. The maximums appear at the positions $(\alpha = 0, \beta = \pi/4)$, $(\alpha = \pi/4, \beta = \pi/2)$, and $(\alpha = \pi/2, \beta = \pi/4)$, all these positions represent the same crystal-orientation $\langle 110 \rangle$. The maximum absolute value of $V''_{\parallel}$ is $|V''_{\parallel}|_{\max} = 1$ corresponding to $\eta = 0, \pi/2$. It means that the optimum polarization direction of initial probe beam is parallel to y'' axis or z'' axis, and the corresponding polarization of the THz field should be parallel to $V''_{\parallel} = (0, 0, 1)$, namely, along the z'' axis.

2.3. Terahertz detection by transceiver

It is possible to individually maximize the generation and detection of the THz electric field in two separate crystals, but when we use the same EO crystal as the THz transceiver described in Ref. [20], the THz electric field generated has the same polarization direction as the THz field applied to the detected crystal; the incident pump beam is the same with the probe beam. The following equation should be satisfied:

$$\eta = \pi/2 - (\varphi - \theta). \quad (16)$$

Inserting Eq. (16) into Eq. (14) and transforming to $x''y''z''$ coordinate system, we can derive the expression of V'' as a function of $\varphi - \theta$. Connecting it with Eq. (6), we can rewrite Eq. (11) as

$$\frac{\Delta I}{I_0} \propto \frac{1}{C} \left[\begin{array}{l} A^2 \left(\frac{3}{4}\sin(4(\varphi-\theta)) - \frac{1}{2}\sin(2(\varphi-\theta)) \right) + AB((3C-3)\cos(4(\varphi-\theta)) + (3C-1)\cos(2(\varphi-\theta))) \\ + B^2(3C-2)\left(\frac{6-3C}{4}\sin(4(\varphi-\theta)) + \frac{4-3C}{2}\sin(2(\varphi-\theta)) \right). \end{array} \right] \quad (17)$$

As shown in Fig. 6, we depict the maximum signal as a function of the crystal-orientation of crystal in the EO transceiver. It should be noted that the signal values have been normalized to the values in Fig. 5. As the THz waves are generated and detected by the same crystal in the transceiver, we lose the flexibility of optimizing the generation and detection, the signal is obviously weakened as shown in the graph. Our calculation reveals that the optimum crystal-orientations are still $\langle 110 \rangle$, whereas the intensity of the signal drops 50% approximately in comparison with the conventional setup with two separate crystals, which agrees well with the conclusion of Ref. [20], however the signal vanishes when the crystal orientation is set to the

⟨111⟩ direction, this conclusion is different from the result in Ref. [20]. We found that there is a small mistake in Eq. (29) of Ref. [20], which results in the mismatch between the two conclusions. After correcting the mistake, the result agrees well with ours, which also verifies our theory. From Ref. [21], only the relative position $\varphi-\theta$ of the polarization of incident pump beam (probe beam) and azimuth of crystal affects the performance of system when the crystal-orientation is fixed, which is the same as the description in Subection 2.1, so we can fix either φ or θ and then modify the other to find the most suitable positions.

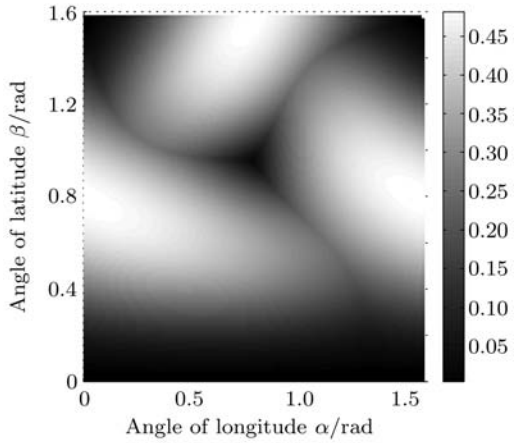


Fig. 6. The normalized signal of EO detection with the EO transceiver as a function of crystal-orientation expressed by longitude α and latitude β.

3. Conclusion

We have presented a full mathematical description of the generation and detection of a THz pulse in zincblende crystals with arbitrary crystal-orientation. Results show that the optimum crystal-orientation for THz generation based on optical rectification is not unique. However, it is reasonable to choose a crystal with ⟨110⟩ orientation in the system for its excellent performance and practicability. We also discussed the EO detection of THz pulses by using THz transceiver. Our theoretical results provided a practical guide to choosing the crystal-orientation for an optimum system performance. The optimal orientation was demonstrated to be ⟨110⟩ and the performance of system will deteriorate considerably when the orientation of the EO crystal used in the transceiver deviates from the ⟨110⟩ orientation. In addition, the detection signal vanished when the crystal-orientation is chosen to be ⟨100⟩ and ⟨111⟩ directions. The polarization of the incident beam can be arbitrary because the azimuth of the EO crystal can be adjusted to meet the optimal demand. All the above conclusions have a great significance to the choice of the crystal-orientation of EO crystal.

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