Investigation of operational characteristics of terahertz-wave parametric oscillators pumped by picosecond based on MgO:LiNbO$_3$ crystal

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**ABSTRACT**

Based on the technology of the non-collinear phase-matching about three-wave interaction in uniaxial crystal, the performance of nonlinear crystal MgO:LiNbO$_3$(MgO:LN) including the phase-matching angles, effective nonlinear coefficient and THz-wave gain as well as its absorption coefficients are theoretically discussed under e-e type phase-matching condition. And an external cavity is developed for terahertz-wave parametric oscillators pumped by picosecond laser (ps-TPOs). For optimizing the ps-TPOs performance, the focusing spot size in MgO:LN crystal, the geometric size of the MgO:LN crystal, the conversion efficiencies, and the stability of the THz-wave generation are designed and calculated. The calculated results provide a comprehensive theoretical basis for the ps-TPOs using difference-frequency generation (DFG) method and optimal performance to generate widely tunable terahertz waves in MgO:LN crystal.

**Keywords:**
Terahertz-wave parametric oscillators
Non-collinear phase-matching
Difference-frequency generation
Picosecond
MgO:LiNbO$_3$ crystal

1. Introduction

The THz waves have been attracted recently because of its wide ranging applications in various fields, including THz imaging [1,2], communications [3], sensing [4], spectroscopy [5,6], and many fields of fundamental and applied physics and technology [7,8]. Since the appearance of a high power near-infrared light source, coherent terahertz waves have been generated successfully using PC antennas [9,10], Q-switched Nd: YAG laser [11,12] or femtosecond ultrashort pulses laser [13].

However, there are few tunable and high-reputation THz-wave sources pumped by picosecond pulsed laser. Then, we have been focusing on picosecond pulsed laser, because picosecond pulsed laser has smaller linewidth than femtosecond pulse and higher-repetition than Q-switched Nd: YAG laser. Furthermore, it has been shown that by mixing two bandwidth-limited picosecond pulses in the DFG scheme [14,15], one could achieve conversion efficiency, which is the same as in the case of femtosecond pulses with the same fluence (or same pulse energy for the focused pump beams). In addition, picosecond pulses’ peak power can be enhanced in a high finesse compact external cavity to overcome the threshold and the spectrum is relatively narrow [16,17]. Therefore, the characteristics of ps-TPOs are analyzed in this paper that organized as follows.

In Section 2, we theoretically discuss the performance of nonlinear crystal MgO:LN including the phase-matching angles, effective nonlinear coefficient and THz-wave gain as well as its absorption coefficients. In Section 3, we develop an external cavity for the doubly resonant ps-TPOs. We also consider optimal focusing spot size; design the geometric size of the MgO:LN crystal; and optimize conversion efficiencies. In the same section, we also discuss the stability of the THz-wave generation using the Runge–Kutta algorithm to simulate the parametric interaction. In Section 4, we draw conclusions.

2. Theoretical performance of nonlinear crystal MgO:LN

Using the 1.064 $\mu$m as one of the pump wavelengths, only e-e type can be phase-matched for the configuration of the THz DFG in MgO:LN crystal, where the first and second letters designate the polarizations for the pump and second (Stokes) beams, while the third letter corresponds to the polarization for the THz waves, respectively. In the stimulated scattering process (as shown in Fig. 1), the generated far-infrared radiation together with the

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Stokes radiations are created parametrically from the pump beam according to the phase-matching condition and energy conservation law

$$\frac{n_e(\lambda_p, \alpha)}{\lambda_p} = \frac{n_e(\lambda_s, \alpha + \theta)}{\lambda_s} + \frac{n_e(\lambda_T)}{\lambda_T}$$  \hspace{1cm} (1)

$$\frac{1}{\lambda_p} = \frac{1}{\lambda_s} + \frac{1}{\lambda_T}$$  \hspace{1cm} (2)

where $\lambda_m$ are the wavelengths with $m = P, S, T$ representing the pump, Stokes, and THz waves, respectively $\theta$ is the phase-matching angle and $\alpha$ is the angle between the pump and optic axis. $n_e(\lambda_p, \alpha)$ and $n_e(\lambda_s, \alpha + \theta)$ are the angle-dependent extraordinary refractive indices of the Stokes and terahertz waves, respectively. And the indices of refraction can be determined by the following traditional dispersion relationships [18]

$$n_s^2 = 1 + \frac{2.245 \lambda^2}{\lambda^2 - 0.01424} + \frac{1.3005 \lambda^2}{\lambda^2 - 0.05313} + \frac{6.897 \lambda^2}{\lambda^2 - 331.33}$$  \hspace{1cm} (3)

$$n_s^2 = 1 + \frac{2.427 \lambda^2}{\lambda^2 - 0.01478} + \frac{1.4617 \lambda^2}{\lambda^2 - 0.05612} + \frac{9.6536 \lambda^2}{\lambda^2 - 371.216}$$  \hspace{1cm} (4)

when the Eqs. (3) and (4) are satisfied, the range of wavelengths $\lambda$ and the temperature $T$ are given in 0.4–5 $\mu$m and $T = 294K$, respectively. Utilizing the refractive-index ellipsoid equation, the indices of refraction $n_e(\lambda_p, \alpha)$ and $n_e(\lambda_s, \alpha + \theta)$ in uniaxial crystals are given by [19]

$$n_e(\lambda_p, \alpha) = \frac{n_{0e} n_0}{\sqrt{n_s^2 \sin^2(\alpha + \theta) + n_p^2 \cos^2(\alpha + \theta)}}$$  \hspace{1cm} (5)

$$n_e(\lambda_s, \alpha + \theta) = \frac{n_{0e} n_0}{\sqrt{n_s^2 \sin^2(\alpha + \theta) + n_p^2 \cos^2(\alpha + \theta)}}$$  \hspace{1cm} (6)

Experimentally, it has been shown that the ordinary and extraordinary refractive indices in MgO:LN do not hold to Eqs. (3) and (4) in the THz domain. The Sellmeier dispersion for the refractive index of MgO:LN crystal in the terahertz region must be formulated using a new dispersion relation model. Assume a THz beam propagating through MgO:LN crystal with complex refractive index $n_{THz} = n(\omega) + ik(\omega)$. In this paper, the extraordinary wave $n_0(\omega)$ whose polarization is parallel to the optical axis (along the z axis) corresponds to the $A_1(z)$ mode, while the ordinary wave $n_0(\omega)$ whose polarization is parallel to the $y$ axis corresponds to the $E(y)$ mode, where $A_1(z)$ and $E(y)$ are both Raman- and infrared-active polar modes. Such a case can be described in the framework of the classical damped harmonic oscillator model [20]

$$\varepsilon(\gamma) = \varepsilon_\infty + \sum_j \left\{ \delta_0 \omega_j^2 - (\omega_{THz}/2\pi)^2 - i(\omega_{THz}/2\pi)^2 \Gamma_j \right\}$$

$$= (n(\omega) + ik(\omega))^2$$  \hspace{1cm} (7)

where $\varepsilon(\gamma)$ is the complex dielectric constant, $\omega_j$, $\delta_0$, and $\Gamma_j$ are the jth eigenfrequency, oscillator strength and damping coefficient of the lowest $A_1$-symmetry phonon mode, respectively, and $\varepsilon_\infty$ is the high-frequency dielectric constant.

According to [21], the refractive indices of ordinary and extraordinary waves in MgO:LN crystal can be calculated in the frequency range from 0.3 to 3 THz (as shown in Fig. 2). It should be noted that since some parameters, such as the lattice vibration parameters, used in this paper are mainly cited from the Refs. [22] and [23]. And the calculated results maybe slightly but negligible discrepancy with others. But we think that the conclusions in our paper still apply. See Fig. 1. The three waves satisfy the e-e type non-collinear phase-matching condition at all times. This leads to the angle-dispersive characteristics of the Stokes and THz waves (as shown in the Fig. 3). Thus, the generation of widely tunable and continuous THz-wave radiations (typically 1–3 THz) can be accomplished simply by changing the angle between the incident pump beam and the resonator axis.

We notice from [24] that the amplitudes of the three optical fields are coupled to one another through effective nonlinear coefficient $d_{eff}$, which is the most important physical quantities dictating the efficient THz parametric conversion. For the configuration introduced above, the effective nonlinear coefficient depends on the azimuth angles $(\alpha, \varphi)$ according to [25] as follows

$$d_{eff}^{e-e} = d_{22} \cos^2 \alpha \cos 3\varphi$$  \hspace{1cm} (8)

where the effective second-order susceptibility $d_{22}$ is about 6.3 ± 0.7 pm/V[26]. Obviously, $d_{eff}^{e-e}$ reaches a maximum value at $\alpha = 0$ corresponding to the phase-matching angle $\theta = 0.45^\circ$ at $\lambda_s = 1.067 \mu$m, $n_0(\omega) = 4.95$. That condition is the primary factor for designing the size of the MgO:LN crystal in Section 3.2.
And the values of effective nonlinear coefficient of MgO:LN crystal at THz-wave wavelengths are shown in Fig. 4.

With the reported paper [22] and [23], the scale of the THz-wave output peak power vs. the crystal absorption in the THz domain are given (as shown in Fig. 5(a)), which is also a key parameter for calculating and designing the length of crystal. The tuning capabilities of the ps-TPOs are also decided by the characteristics of the THz-wave parametric gain \( g_{\text{THz}} \) as well as its absorption loss inside the crystal. According to the Refs. [12] and [27], the analytical expression of the exponential gain for the THz waves is given by

\[
g_{\text{THz}} = g_s \cos \varphi = \frac{\alpha_{\text{THz}}}{2} \left[ 1 + 16 \cos \varphi \left( \frac{g_0}{\alpha_{\text{THz}}} \right)^{1/2} - 1 \right] \tag{9}
\]

where \( \varphi \) denotes the phase-matching angle between the pump and THz waves; \( g_0 \) is the effective parametric gain coefficient containing the effect of lattice vibration. In cgs units, they are defined as follows

\[
g_0 = \frac{\pi \omega_0 \alpha_{\text{THz}} P_p}{2 c^2 n_p^2 (\alpha_p + \alpha) n_p^2 (\alpha + \theta) n_{\text{THz}} (\omega_{\text{THz}}) \alpha_{\text{THz}}^2} \left( \frac{d^2}{\omega^2} + \sum_j \frac{S_j \omega^2 d_j^2}{\omega^2 - \omega_{\text{THz}}^2} \right) \propto \sqrt{\omega_0} \alpha_{\text{THz}} I_p \tag{10}
\]

\[
\alpha_{\text{THz}} = \frac{2 \omega_{\text{THz}}}{c} \frac{\text{Im} \sqrt{\varepsilon(\gamma)}}{\omega_{\text{THz}}^2} \frac{\text{Im}(\varepsilon_{\infty}) + \sum S_j \omega^2}{\omega^2 - (\omega_{\text{THz}}/2\pi)^2 - i(\omega_{\text{THz}}/2\pi)^2 I_j}^{1/2} \tag{11}
\]

where \( I_p = P_p/\pi r^2 \) denotes the pump intensity. The value of the effective third-order susceptibility \( d_{33} \) is 25.2 pm/v [28]. The nonlinear coefficients \( d_{33}^p = 16 \pi d_{33} [12] \) and \( d_{33}^c = -18 \pi d_{33} [29] \) represent second- and third-order nonlinear optical process, respectively. \( \alpha_{\text{THz}} \) has a relatively small value in the low-frequency region but it quickly increases as the THz frequencies are increased (see Fig. 5(a)). Therefore, in the high-frequency region, \( \alpha_{\text{THz}} \) exceeds the contribution of \( g_0 \) so that the gain coefficient starts to decrease (see Fig. 5(b)). The decrease in the linewidth \( \Gamma_j \) of the lowest \( \alpha_{\text{THz}} \)-symmetry phonon mode [30] makes the major contribution to the enhancement at low temperature, because \( \alpha_{\text{THz}} \) is nearly in proportion to \( \Gamma_j^{1/2} \) (Eq. (11)). The reduced linewidth reduces the absorption coefficient \( \alpha_{\text{THz}} \) at THz frequencies, enhancing the parametric gain \( g_{\text{THz}} \), which is a monotonically decreasing function of the absorption coefficient (Eq. (9)). For the analysis above, the picosecond pulsed laser being the pump source has smaller linewidth than the ns-TPOs, which could effectively reduce the absorption coefficient and improve the conversion efficiency.

Fig. 5(b) shows the calculated parametric gain \( g_{\text{THz}} \) for MgO:LN at typical pump intensities, which in the frequency up to 3 THz can be easily achieved in the order of several cm\(^{-1}\). It is also possible to increase the parametric gain by increasing the pump intensity with the center frequency of the THz waves from the low-frequency region into high frequency region, or by using a shorter wavelength pump source because the gain is a monotonically increasing function of \( g_0 \) which is proportional to \( \omega_{\text{THz}}^{1/2} = (\omega_0 - \omega)^{1/2} \) (Eq. (10)).

3. The operation characteristics of terahertz-wave parametric oscillators

3.1. The development of external cavity for the ps-TPOs in MgO:LN crystal

Fig. 6 shows a schematic of the setup for the doubly resonant THz parametric oscillators with MgO:LN crystal. The picosecond pulses are delivered using a mode-locked 1.064 μm laser that provides 10 ps pulses width with a maximum average output of 9 W and a repetition rate of 100 MHz. The pump beam is divided into two beams using beam splitter (BS), so we can display the pulses width which is an important parameter for optimizing optical-to-terahertz photon conversion efficiency (in Section 3.4). And mode-matching lenses (l1, l2) coupled the collimate the other
pump beam into the external bow-tie ring cavity with two planar mirrors (M1, M2) and two curved mirrors (M3, M4), which mirror M2 is mounted on a piezoelectric transducer (PZT) using photo-detector and feedback electronics to actively-stabilized the cavity length. The generated THz waves emit at 65° from the pump beam direction. After leaving MgO:LN crystal, the THz waves are collimated by cylindrical lens (CL) made of poly(methylmethacrylate) (PMMA) [31] to compensate the different beams divergences and focus the THz-wave radiations, then measured with detect systems.

3.2. Design the size of the MgO:LN crystal

Actually the optimal size of the MgO:LN crystal is designed by following the three steps: initially confirm the range of crystal length's value; secondly calculate the value of optimal crystal length; and then design the idiographic value of crystal size.

(i) According to [16], we can choose reasonable order of magnitude for the crystal length $L$, depending on the condition $L \propto 1/\alpha_{THz}$, where $\alpha_{THz}$ has a relatively small value in the low-frequency region but quickly increases as the THz frequencies are increased. From the reported paper on the experimental research [17] [32] the results of the THz-wave output power have the maximum values in the frequency domain $\omega_{thz} = 0.8–1.2$ THz corresponding to the value of $\alpha_{THz} = 0.18–1.2$ cm$^{-1}$ (as shown in Fig. 5(a)). Hence the range of crystal length $L$ is confirmed on 10–50 mm.

(ii) The optimal crystal length can be achieved with such calculation where Huang's paper [33] expresses the theoretical analysis using the Runge–Kutta algorithm to solve the three-wave coupled equations. In Section 3.5, we will discuss the details of the stability of THz-wave generation using the same method. Fig. 7 shows the calculated THz-wave power as a function of the MgO:LN length at $\omega_{THz} = 1$ THz, $\lambda = 300$ μm with $\alpha_{THz} = 5.3$ pm/μm (Fig. 4(b)), $I_p(\max) = 10$ MW/cm$^2$, $I_2(\max) = 0.5$ MW/cm$^2$, $\lambda_p = 1064$ nm, $\lambda_s = 1067$ nm (Fig. 3), $n_e(\lambda_p, \alpha) = 2.2288$ (Eq. (5)), $n_e(\lambda_s, \alpha + \theta) = 2.2284$ (Eq. (6)), $n_e(\alpha) = 4.95$ (Fig. 1), $\alpha_{THz} = 0.61$ cm$^{-1}$ (Fig. 5(a)). The THz-wave intensity does not increase monotonically with the length, but saturates above 40 mm and decreases above 45 mm, due to the absorption of MgO:LN in the THz-wave region. As a result of the above calculations, a 40 mm long MgO:LN crystal is used for the experiment.

(iii) To overcome the problems that the heavy absorption loss in the THz domain, the angled surface coupler's method is preferred to couple the generated THz waves. And the process technology of crystal and detect systems' limitations are also considered. In Section 2, we notice from Eq. (8) that $d_{\text{eff}}\varphi$ reaches a maximum value at $\varphi = 0°$ corresponding to the phase-matching angle $\theta = 0.40°$. Inside the MgO:LN, the angle $\varphi$ between the pump and Stokes beams depicted in Fig. 1 is given by $\varphi = \alpha \cos(\kappa_2 - \kappa_2)/2k_0 \times k_1$ where $k_0 = 2\pi n_2(\lambda_p, \alpha)/\lambda_p$, $n_2 = 2\pi n_2(\lambda_s, \alpha + \theta)/\lambda_s$, $k_2 = 2\pi n_2/\lambda$. With the Eq. (2), the corresponding angle $\varphi = 64°$. Then the generated THz waves emit at $\theta + \varphi = 65°$ degrees from the pump beam direction where the cutting-off sectional orientation must be perpendicular to the THz-wave direction, hence $\beta = 90° - (\theta + \varphi) \approx 25°$. With the input beam at the entrance facet of the MgO:LN $\omega_{\text{optimal}} = 430 \mu$m (calculated in Section 3.3), the value of the Lmin (as shown in Fig. 1) is 3.8 mm according to the geometric optic's principle. Finally a 5 mm thick MgO:LN crystal is cut to a dimension of 40 mm (L) × 36.2 mm (L1) × 5 mm (W) × 3.8 mm (W1) × 5 mm (T).

3.3. Optimal focusing spot size

Practicality the reasonable focusing spot size is an important parameter for choosing the commercial crystal and designing the external bow-tie ring cavity, which is optimized by following three steps: firstly calculate the minimum focusing spot size; posteriorly take care for the damage threshold with the theoretical focusing spot size; and then get the details of the optical component arrangement corresponding to the optimum spot size.

(i) When pump beam waist $\omega_{\text{min}}$ is too small, THz output extends over a larger span of angles $\theta$ to the normal of the crystal; when $\theta$ exceeds the total internal reflection angle $\theta_{\text{max}}$ of the material, THz-wave transmission falls to zero. This leads to the condition $2\theta_{\text{max}} > \sqrt{2(\lambda_{\text{THz}}/\pi n_{THz})\omega_{\text{min}}}$. For MgO:LN, for example $\theta_{\text{max}} = 12°$, and for $\lambda_{\text{THz}} = 300$ μm, $n_{THz} = 4.95$, this corresponds to $\omega_{\text{min}} > 65$ μm.

(ii) When the pump pulses width are on the order of 10ps and 10 ns, MgO:LN crystals' damage threshold are almost above 0.8 Gw/cm$^2$ [34] and 25 Mw/cm$^2$ [34,35]. In our experiment, the picosecond's laser provides 10 ps pulses with a maximum output power of 9 W and a repetition rate of 100 MHz. With above calculated the minimum spot size beam $\omega_{\text{min}}$, the pump intensity maximum value is 10 Mw/cm$^2$, which is less than the MgO:LN crystals' damage threshold value.

(iii) In the near field approximation, the loose and diffraction can be neglected. Following Boyd-Kleinman focusing function Ch.5 of [36], the DFG case is considered, which the optimum condition for focusing is that the confocal parameter $b_{\text{cp}}$ for the output THz beam is a half of the crystal length $L(\xi = L/b_{\text{cp}} = 2)$.
which the value of the crystal length \( L \) is 40 mm calculated in Section 3.2. The diameter of the fundamental beam at the center of the MgO:LN crystal is approximately \( \omega_{\text{optimal}} = 430 \mu m \) \((\omega_{\text{optimal}} = \sqrt{\lambda_{\text{THz}}L}/2\pi r_{\text{THz}}) \), which is focused on the center of the MgO:LN crystal by the two curve mirrors (M3, M4). The optical arrangement of the mirrors and the crystal is determined by the ABCD matrix. And the details of optical arrangement are shown in Fig. 8, corresponding to the optimal focusing spot size \( \omega_{\text{optimal}} \). The cavity length is \( \sim 1.5 \) m in length with a round-trip time equal to the period between pump laser pulses.

3.4. Optimize conversion efficiencies

Primarily we refine the formula of the THz-wave output power under mismatching condition, meanwhile the pump and Stokes beams absorption coefficients are eliminate from the formula, furthermore the optical-to-terahertz conversion efficiency is defined. And then the optimal performances are considered for improving conversion efficiencies including optical-to-terahertz conversion efficiency and photon conversion efficiency.

In experiment, the phase-matching angles are observed as the MgO:LN crystal is carefully rotated utilizing motorized translation stages. Since the ideal PM condition cannot be satisfied, according to the expression of the THz output power for the DFG [37,38], a parametric gain still exists for the phase mismatch function \( \sin^2(\Delta kL/2) \) where \( \Delta k \) is the value of the wave vector mismatch. Even the MgO:LN crystal always has anomalously larger absorption coefficients in the near-infrared domain (1–2 \( \mu \)m), the pump and Stokes beams wavelengths are tightly approximated, where the absorption coefficients of the pump and Stokes beams are abbreviatory, and \( \Delta \alpha \) is defined by \( \Delta \alpha = |\alpha_p - \alpha_S - \alpha_{\text{THz}}| = |\alpha_{\text{THz}}| \). Only considering the absorption of the terahertz waves \( \alpha_{\text{THz}} \) in the process of DFG in MgO:LN crystal, we rewrite the expression of the output power of terahertz waves as follows

\[
P_{\text{THz}} = \frac{2\omega_{\text{THz}}^2}{\epsilon_0 c^2 1/\epsilon_0^2} (d_{\text{eff}}^{\text{ee}})^2 L^2 \left( \frac{P_p P_S}{\pi r^2} \right) T_1 T_2 T_3 S \]

\[
S = \exp(-\alpha_{\text{THz}} L) \times \left( 1 + \exp(-\alpha_{\text{THz}} L) - 2 \epsilon \cos(\Delta k L) \right)
\]

where \( \omega_{\text{THz}} \) is the frequency of the THz waves. \( d_{\text{eff}}^{\text{ee}} \) can be calculated from Eq. (8), \( L \) is the length of the MgO:LN crystal. The \( P_p \) and \( P_S \) are input peak powers of the pump and Stokes. \( T_1, T_2 \) and \( T_3 \) are the Fresnel transmission coefficients, given by \( T_{1,2,3} = \sqrt{4\eta_p S \text{THz}/(\eta_p S + 1)} \).

\( \epsilon_0 \) is the vacuum permittivity. \( c \) is the speed of light in vacuum. \( r \) is the radius of the focus spot in MgO:LN crystal. With these calculational parameters such as phase-matching angles, the optical-to-terahertz conversion efficiency can be expressed in the form

\[
\eta = \frac{2\omega_{\text{THz}}^2 (d_{\text{eff}}^{\text{ee}})^2 L^2}{\epsilon_0 c^2 1/\epsilon_0^2} \left( \frac{P_p P_S}{\pi r^2} \right) T_1 T_2 T_3 S \]

(13)

To maximize the conversion efficiencies, we need to consider three aspects on the optimal performances:

(i) By analyzing the focusing spot size as a function of optical-to-terahertz conversion efficiency (as shown in Fig. 9), the optimizing performance could be easily achieved by adjusting the positions of two convex lenses used to focus two pump beams, which the limitations have been discussed in Section 3.2.

(ii) Furthermore, an effective other way to enhance the optical-to-terahertz conversion efficiency is to increase the power density of the pump beams, which is proportional to \( \sqrt{P_p P_S} \) (Eq. (13)). And mode-matching lenses (1, 2) are also used to change the spot size for varying the power density outside the cavity (as shown in Fig. 6).

(iii) During the experimental operation, it is highlight that the relationship between pulse width, repetition rate and THz-wave output or conversion efficiencies are explored, comparing with describing traditional OPO model parameters’ relationship. To the best of our knowledge, only the paper [39] is the first report on the strong saturation in the conversion efficiency for the THz waves generated by DFG, and the paper [40] is the first report on the THz-output power formula involving the pulse width and repetition rate, but the relationship between pulse width, repetition rate and THz-wave output or conversion efficiencies are not clearly given. In Ref. [39], assuming the \( P_p \gg P_S \), the photon conversion efficiency for the THz generation inside the MgO:LN crystal can be obtained:

\[
\eta_p = \eta_{\text{max}} \sin^2 \left( \frac{\pi}{2} \right) \sqrt{\frac{P_{\text{ave}}}{P_{\text{opt}}}}
\]

(14)

where \( \eta_{\text{max}} = S_T/S_p \) is the maximum conversion efficiency with \( S_T \) and \( S_p \) being the areas of the THz radiation and input pump beam at
1.064 μm and $P_{\text{ave}}$ is the average input pump power at 1.064 μm. In Eq. (14), $P_{\text{opt}}$ is an optimal power under assuming conditions for calculating the Eq. (12):

$$P_{\text{opt}} = \frac{c\varepsilon_0 n^2_p(\lambda_p, \alpha) n^2_S(\lambda_S, \alpha + \theta) n^2_{THz}(\lambda_{THz}, \delta_0) \gamma T(\pi/2)^2 R}{16(\delta_{\text{eff}})^2 L^2 T_1 T_2 T_3}$$  (15)

where $\tau$ and $R$ are the pulse duration and the repetition rate. With the Eqs. (14) and (15), the relationship between pulse width, repetition rate and THz-wave output the photon conversion efficiency are shown in Fig. 10, which the optimal performance could be achieved easily by changing the pulse width and repetition rate. The following curve for typical commercial mode-locked ps-lasers (High Q Laser, Model number: picotRAIN, 7.5 ps, >10 W, 50 MHz; Photronics Industries, Model number: ps-1064-10, 20–25 ps, 10 W, 80 MHz) have been included to compare the effect of the pulse width, repetition rate on the photon conversion efficiency.

3.5. The stability of THz-wave generation

For the reason of optical-to-terahertz conversion efficiency and THz-wave output power are lower, the detect systems are sensitive in fluctuating and challenging for collecting the THz signals. So the published papers focusing on the experimental research are seldom referring the stability of the THz-wave generation where only Huang’s paper [33] expresses the correlative theoretical analysis. In Section 3.2, we have been using the Runge–Kutta algorithm to achieve the optimal crystal length, which the index of the stability can also be discussed under initialization parameters setting for ps-TPOs. And the calculated results are given by:

(i) From Fig. 5(b), it is shown that the THz-wave gain coefficients can be enhanced by increasing the power density, which is also a key parameter for the stability. Curves of THz-wave output intensity dependence on the crystal length are given in Fig. 11, which are respected to different pump intensities stepwise decreasing by 0–10% of the first value with the same Stokes intensity.

(ii) From Eq. (9), we notice that the Stokes beam gain coefficients are proportional to THz-wave gain coefficients. So the effect of Stokes intensity fluctuations on the stability of the THz output is also an important factor whose power can be monitored after mirror M1 and converted into Stokes intensity. And the fluctuations of the Stokes intensity can be achieved by rotating the motorized translation stages. Curves of THz-wave output intensity dependence on the crystal length are given in Fig. 12, which are respected to different Stokes intensities stepwise decreasing by 0–10% of the first value with the same pump intensity.

Comparing with the Figs. 11 and 12, the THz-wave output intensity is sensitive to the pump changes around the saturation peak point. Hence the THz-wave output stability is primarily determined by the pump stability. Furthermore the details can be clearly seen from Fig. 12. With 10% Stokes variation, the THz output changes are less than that in the unsaturated region. Thereby the optimum stability can be possibly achieved. For example, once the crystal length is given, one can vary the Stokes intensity to locate saturation region, similarly the optimal operation can be used for varying the pump intensity.

4. Conclusions

Primarily we calculate the performance of nonlinear crystal MgO:LN including the phase-matching angles, effective nonlinear coefficient and THz-wave gain as well as its absorption coefficients under e-ee type phase-matching condition. According to these calculational parameters, we can design the size of the crystal, and calculate the conversion efficiency. Posteriorly the optical component of the external cavity is devised by the ABCD matrix corresponding to the optimal focusing spot. And then the Runge–Kutta algorithm is used for analyzing the stability of the THz-wave generation. In our next step, we will present in detail further experimental relative results (paper in preparation) in order to enlarge
and improve the basis for theoretical work on the optimal performance. Based on the analysis and simulation, the ps-TPOs can efficiently achieve more THz-wave output. And this method could be a useful way to generate the widely tunable THz waves.

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