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Calculations of optimum phase match parameters for the biaxial crystal KTiOPO₄

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The expression for the optimum phase matching angle for the biaxial crystal KTiOPO₄ (KTP) is presented and numerically calculated. The theoretical effective nonlinear coefficient, walk-off angle, and conversion efficiency are determined. The results provide some theoretical and practical guidance for optimum operation of biaxial crystals, with specific numerical calculations for KTP.

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Phase matched second harmonic generation (SHG) in biaxial crystals has been discussed by Hobden.1 Zumsteg et al.2 and Liu et al.3,4 discussed some of the phase matching properties of KTiOPO₄ (KTP). The literature to date has presented results of phase match calculations and experiments which show the possible phase match angles. In addition to giving the details of such calculations, we have derived an expression for the effective nonlinear coefficient \(d_{eff}\) of a biaxial crystal and have calculated this coefficient numerically for KTP for both Type I and Type II doubling. This, the optimum, phase matching direction was determined, and the theoretical walk-off angles, influence of mismatching and critical crystal length were calculated. The results provide some theoretical and practical guidance for optimum operation of a biaxial crystal.

PHASE MATCH ANGLES

The refractive indices \(n_w\) and \(n_{2w}\) of the fundamental and harmonic frequencies at an arbitrary incident direction must obey the following equations, respectively,

\[
k_{x}^{2}/(n_{w}^{2} - n_{x,w}^{2}) + k_{y}^{2}/(n_{w}^{2} - n_{y,w}^{2}) + k_{z}^{2}/(n_{w}^{2} - n_{z,w}^{2}) = 0,
\]

\[
k_{y}^{2}/(n_{2w}^{2} - n_{x,2w}^{2}) + k_{x}^{2}/(n_{2w}^{2} - n_{y,2w}^{2}) + k_{z}^{2}/(n_{2w}^{2} - n_{z,2w}^{2}) = 0,
\]

where \(k_{x}^{2} = \sin \theta \cos \phi, k_{y} = \sin \theta \sin \phi, \) and \(k_{z} = \cos \theta.\) Here, \(\theta\) is the angle between the wave normals and the \(z\) axis, and \(\phi\) is the angle from the \(x\) axis in the \(xy\) plane. \(n_{x,w}, n_{y,w}, n_{z,w}, n_{x,2w}, n_{y,2w}, n_{z,2w}\) are the three principal refractive indices of fundamental and harmonic waves, respectively, at a given temperature.

Equations (1) and (2) can be written as

\[
x_{1}^{2} + B_{1}x_{1} + C_{1} = 0,
\]

\[
x_{2}^{2} + B_{2}x_{2} + C_{2} = 0,
\]

by letting

\[
x_{1} = n_{x,w}^{2}, \quad x_{2} = n_{x,2w}^{2},
\]

\[
B_{1} = \left[ -k_{x}^{2}(b_{1} + c_{1}) - k_{y}^{2}[a_{1} + c_{1}] - k_{z}^{2}(a_{1} + b_{1}) \right],
\]

\[
C_{1} = \left[ k_{x}^{2}b_{1}c_{1} + k_{y}^{2}a_{1}c_{1} + k_{z}^{2}a_{1}b_{1} \right],
\]

\[
B_{2} = \left[ -k_{x}^{2}(c_{2} + b_{2}) - k_{y}^{2}[a_{2} + c_{2}] - k_{z}^{2}(a_{2} + b_{2}) \right],
\]

\[
C_{2} = \left[ k_{x}^{2}b_{2}c_{2} + k_{y}^{2}a_{2}c_{2} + k_{z}^{2}a_{2}b_{2} \right],
\]

where

\[
a_{1} = n_{x,2w}^{-2}, \quad b_{1} = n_{y,2w}^{-2}, \quad c_{1} = n_{z,2w}^{-2},
\]

\[
a_{2} = n_{x,2w}^{-2}, \quad b_{2} = n_{y,2w}^{-2}, \quad c_{2} = n_{z,2w}^{-2}.
\]

Equations (1a) and (2a) can be solved for \(n_{x,2w}, n_{y,2w}, n_{z,2w}\) for Type I and II doubling.

\[
\sqrt{B_{1}^{2} + 4C_{1}} = \sqrt{-B_{2} + \sqrt{B_{1}^{2} - 4C_{1}}},
\]

\[
\sqrt{B_{2}^{2} + 4C_{2}} = \sqrt{-B_{1} + \sqrt{B_{2}^{2} - 4C_{2}}},
\]

As \(i = 1, \) or \(2,\) the symbols under the square root sign take on plus or minus values, respectively.

It is obvious that \(n_{x,2w} > n_{y,2w}\) and \(n_{y,2w} > n_{z,2w}.\) For Type I and II phase matching, \(n_{x,2w} = n_{y,2w} = 1/2(n_{x,2w} + n_{y,2w}) = n_{z,2w},\) respectively. Therefore, for Type I,

\[
\frac{1}{2} \sqrt{B_{1} + \sqrt{B_{1}^{2} - 4C_{1}}} + \frac{1}{2} \sqrt{B_{2} + \sqrt{B_{2}^{2} - 4C_{2}}} = \frac{\sqrt{\sqrt{B_{1} + \sqrt{B_{1}^{2} - 4C_{1}}} + \sqrt{B_{2} + \sqrt{B_{2}^{2} - 4C_{2}}}}}{\sqrt{-B_{1} + \sqrt{B_{1}^{2} - 4C_{1}}}},
\]

and for Type II,

\[
\frac{1}{2} \sqrt{B_{1} + \sqrt{B_{1}^{2} - 4C_{1}}} + \frac{1}{2} \sqrt{B_{2} + \sqrt{B_{2}^{2} - 4C_{2}}} = \frac{\sqrt{\sqrt{B_{1} + \sqrt{B_{1}^{2} - 4C_{1}}} + \sqrt{B_{2} + \sqrt{B_{2}^{2} - 4C_{2}}}}}{\sqrt{-B_{2} + \sqrt{B_{2}^{2} - 4C_{2}}}}.
\]

Equations (7) and (8) can be used to calculate all possible phase matching directions in one quadrant for Type I and Type II.

From a curve fit of Zumsteg's data for a KTiOPO₄ (KTP) crystal at \(\omega = 1.064 \mu\) and \(2\omega = 0.532\) at room temperature, we have

\[
n_{x,2w} = 1.738, \quad n_{y,2w} = 1.747, \quad n_{z,2w} = 1.833,
\]

\[
n_{x,2w} = 1.779, \quad n_{y,2w} = 1.791, \quad n_{z,2w} = 1.889.
\]

The phase matching angles \((\theta, \phi)\) for Type I and II doubling shown in Fig. 1 are the results of numerical solutions to Eqs. (7) and (8) using the given indices of refraction. It is important to note that changes in the third decimal place of the refractive index values can appreciably change the calculated phase match angle.

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EFFECTIVE NONLINEAR COEFFICIENT

The three components of an electric field at any wave normal directions \((k_x, k_y, k_z)\) satisfy the following equations,

\[
\begin{aligned}
&n_{x,\text{max}}^2 - n_{x,\text{max}}^2(1 - k_z^2)]E_{x,\text{max}} + n_{x,\text{max}}^2 k_x k_y E_{y,\text{max}} + n_{x,\text{max}}^2 k_x k_z E_{z,\text{max}} = 0, \\
&n_{x,\text{max}}^2 k_x k_y E_{y,\text{max}, i} + [n_{x,\text{max}}^2 - n_{x,\text{max}}^2(1 - k_z^2)]E_{y,\text{max}, i} = 0, \\
&n_{x,\text{max}}^2 k_x k_z E_{z,\text{max}, i} + [n_{x,\text{max}}^2 - n_{x,\text{max}}^2(1 - k_z^2)]E_{z,\text{max}, i} = 0,
\end{aligned}
\]  

(9)

where \(m = 1\) and \(2\) indicate fundamental and second harmonic, and \(i = 1, 2\), indicate the two possible values of the refractive indices [as in Eqs. (5) and (6)].

From Eq. (9) and the values of \(\theta\) and \(\phi\) just calculated, we can get three components of \(E_{x,\text{max}}\) and \(E_{2x,1}\) (for Type I) and \(E_{x,1}\), \(E_{x,2}\), and \(E_{2x,1}\) for (Type II) for each pair of phase match angles, \(\theta\) and \(\phi\) \((k_x, k_y, k_z)\). We can then find the direction cosine of each electric field. The fields are expressed as

\[
E_{x,\text{max}}(\cos \alpha_{\text{max}, i}, \cos \beta_{\text{max}, i}, \cos \gamma_{\text{max}, i}).
\]

The second-order polarization \(p(2\omega)\) produced by the interaction of two applied electric fields \(E_j(\omega)\) and \(E_k(\omega)\) in a nonlinear optical medium is given by

\[
p(2\omega) = a_j a_k E_j(\omega)E_k(\omega).
\]

(10)

For Type I phase matching we have

\[
d_{ij}(I) = a_i a_j d_{jk},
\]

\[
= 2d_{15} \cos \alpha_{2x,1} \cos \alpha_{x,2} \cos \gamma_{\text{max},2}
\]

\[
+ 2d_{24} \cos \beta_{2x,1} \cos \beta_{x,2} \cos \gamma_{\text{max},2}
\]

\[
+ d_{31} \cos \gamma_{2x,1} \cos \alpha_{x,2} \cos \gamma_{\text{max},2}
\]

\[
+ d_{32} \cos \gamma_{2x,1} \cos \beta_{x,2} \cos \gamma_{\text{max},2}
\]

\[
+ d_{33} \cos \gamma_{2x,1} \cos \gamma_{\text{max},2}.
\]

(11)

Similarly, the effective nonlinear coefficient for Type II is given by the expression

\[d_{ij}(II) = a_i a_j d_{jk},\]

\[d_{ij}(II) = d_{15} \cos \alpha_{2x,1} \cos \alpha_{x,2} \cos \gamma_{\text{max},2}
\]

\[+ d_{24} \cos \beta_{2x,1} \cos \beta_{x,2} \cos \gamma_{\text{max},2}
\]

\[+ d_{31} \cos \gamma_{2x,1} \cos \alpha_{x,2} \cos \gamma_{\text{max},2}
\]

\[+ d_{32} \cos \gamma_{2x,1} \cos \beta_{x,2} \cos \gamma_{\text{max},2}
\]

\[+ d_{33} \cos \gamma_{2x,1} \cos \gamma_{\text{max},2}.
\]

(12)

In terms of the definition of the effective nonlinear coefficient for Type I, we have

\[d_{ij}(I) = a_i a_j d_{jk},\]

\[= 2d_{15} \cos \alpha_{2x,1} \cos \alpha_{x,2} \cos \gamma_{\text{max},2}
\]

\[+ 2d_{24} \cos \beta_{2x,1} \cos \beta_{x,2} \cos \gamma_{\text{max},2}
\]

\[+ d_{31} \cos \gamma_{2x,1} \cos \alpha_{x,2} \cos \gamma_{\text{max},2}
\]

\[+ d_{32} \cos \gamma_{2x,1} \cos \beta_{x,2} \cos \gamma_{\text{max},2}
\]

\[+ d_{33} \cos \gamma_{2x,1} \cos \gamma_{\text{max},2}.
\]

FIG. 2. Effective nonlinear coefficient \(d_{ij}\) vs \(\phi\) plotted on the first quadrant.
Using Eqs. (12) and (14) for every possible phase matching direction \( \delta'_{\text{I}} \) and \( \delta'_{\text{II}} \) can be calculated. Figure 2 is a plot of the effective nonlinear coefficient \( \delta'_{\text{II}} \) for Type I and II doubling as a function of \( \delta \). The phase matching direction having the maximum effective nonlinear coefficient among all possible phase matching directions is termed the optimum phase matching direction.

**WALK-OFF ANGLE**

Since \( D, k, E, \) and \( S \) are given by Zumsteg, we can calculate \( S_{1w,1}, S_{1w,2}, S_{2w,1} \) for all directions, where \( D, k, E, \) and \( S \) are the dielectric displacement, wave, electric field, and pointing vectors, respectively.

The calculated walk-off angles (the biggest angle difference between \( S_{1w,1}, S_{1w,2}, S_{2w,1} \)) for Type II are plotted in Fig. 3. The walk-off angle \( W \) in the optimum phase matching direction has a minimum value, which in this case is 0.262°.

**CONVERSION EFFICIENCY**

The output power of the second harmonic is given by

\[
P_2 = P(2\omega) = \eta_{\text{SHG}} \left[ \sin(\Delta k/2l_c)/(\Delta k/2l_c) \right]^2 P(\omega)
\]

where \( \Delta k = \omega \Delta n/c, l_c \) is the crystal length, \( P(\omega) = P_1 \) is the fundamental wave power, \( \eta_{\text{SHG}} \) is the SHG conversion coefficient and \( \eta_m \) is the mismatching coefficient. In the ideal phase matching case \( \eta_m = 1 \). Then

\[
P_2 = \eta_{\text{SHG}} P_1.
\]

Using Eqs. (12) and (14) for every possible phase matching direction \( \delta'_{\text{I}} \) and \( \delta'_{\text{II}} \) can be calculated. Figure 2 is a plot of the effective nonlinear coefficient \( \delta'_{\text{II}} \) for Type I and II doubling as a function of \( \phi \) using nonlinear coefficients given by Zumsteg. The maximum \( \delta'_{\text{II}} \) occurs at \( \theta = 90°, \phi = 21.3° \) for Type II phase matching. In this case

\[
\delta'_{\text{II}}(\text{max}) = d_{15} \cos \alpha_{2w,1} (\cos \alpha_{1v,1} \cos \alpha_{1v,2}) + d_{24} \cos \beta_{2w,1} (\cos \beta_{1v,1} \cos \gamma_{1v,2}) = 0.974 d_{24} = 17.7 \times 10^{-9}
\]

c.s.u.
there is mismatching due to misalignment or temperature change, \( \eta_m < 1 \). Now we consider individually \( \Delta \theta \) and \( \Delta \phi \), which are small angle deviations from their ideal values \( \theta_0 \) and \( \phi_0 \) (here \( \theta_0 = 90^\circ \) and \( \phi_0 = 21.3^\circ \)). For Type II,

\[
\Delta n = n_{2\omega,1} - 1/2(n_{\omega,1} + n_{\omega,2}).
\]

From Eqs. (5) and (6), then,

\[
\Delta k = \left( \frac{\omega}{c} \right) \times \left( \frac{\sqrt{2}}{\sqrt{-B_2 + \sqrt{B_2^2 - 4C_2}} - \frac{1}{\sqrt{2\sqrt{-B_1 + \sqrt{B_1^2 - 4C_1}}}} - \frac{1}{\sqrt{2\sqrt{-B_1 - \sqrt{B_1^2 - 4C_1}}}}} \right).
\]

The results of calculating \( \eta_m \) vs \( \Delta \theta \) and \( \Delta \phi \) (assuming the thermal mismatch of a cooled cavity is negligible) are shown in Fig. 4. We note that the curves are not symmetric relative to \( \Delta \theta \) or \( \Delta \phi = 0 \), and the influences of \( \Delta \theta \) and \( \Delta \phi \) are different.

At \( (\Delta k l_c)/2 = \pi/2 \), we get the angular acceptance angles,

\[
\Delta \theta_{\text{max}} = -7^\circ \sim 7.2^\circ,
\]

\[
\Delta \phi_{\text{max}} = -7.8^\circ \sim 11^\circ \text{ [at } l_c = 3.7 \text{ mm]},
\]

and

\[
\Delta \theta_{\text{max}} = -3.3^\circ \sim 4.2^\circ,
\]

\[
\Delta \phi_{\text{max}} = -4.7^\circ \sim 4.8^\circ \text{ [at } l_c = 10 \text{ mm]}.
\]

Then we can calculate a corresponding critical crystal length \( l_c \) vs small \( \Delta \theta \) or \( \Delta \phi \), respectively. \( l_c \) is defined as the crystal length which satisfies \( (\Delta k l_c)/2 = \pi/2 \) at each given \( \Delta \theta \) and \( \Delta \phi \). These are shown by the dashed lines in Fig 4.

**SUMMARY**

In terms of the above analysis and calculation, the optimum operation of a KTP crystal for SHG at 1.06 \( \mu \) is as follows: the phase matching direction is Type II operation in \( x-o-y \) plane with \( \theta = 90^\circ \), \( \phi = 21.3^\circ \). Its effective nonlinear coefficient, \( d_{eff}(II) = 17.7 \times 10^{-9} \) e.s.u. Its walk-off angle is 0.262\(^\circ\). As noted, slightly different values of the refractive indices change the numerical results.

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