Modelling and Simulation for the Electro-optic Characteristics of BaTiO₃ Crystal Film Waveguide with Complementary Push-pull Polarization Modulations

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Abstract. BaTiO₃ crystal films, possessing the advanced electro-optic (EO) properties, have been activating a broad interest in research and development of EO modulators for optic-fibre communications. However, the accurate measurements for the key physical parameter, the EO coefficient, is still at unoriented state. In this work, a BaTiO₃ crystal film is grown on a magnesium oxide (MgO) crystal substrate and a device structure having an ultrahigh two-dimensional (2D) optic-electric field interaction is designed to conduct the synchronous measurements for the EO coefficient $r_{51}$ and the birefringence $b_{eo}$ of the BaTiO₃ crystal film with an intra-guide push-pull modulation of linear polarization. As a result, the average values of $570\pm2\text{pm/V}$ and $-0.0135\pm0.0007$ of $r_{51}$ and $b_{eo}$ are obtained, respectively. Furthermore, a theoretical model for analysing the measurement accuracies of $r_{51}$ and $b_{eo}$, and the accuracy dependences on the drive voltage and optic-electric interaction efficiency are studied, leading to an efficient way to developing the high-speed BaTiO₃ crystal film EO modulators.

1. Introduction
In the past decades, optical communication network has developed rapidly, and the parallel research and development of devices, structures and systems have been carried out with the goal of 5G optical network. Especially in recent years, integrated optical devices and modules based on waveguide technology have been widely developed and applied, and the data rate and capacity of optical communication systems are also increasing rapidly[1-4]. Winzer et al., a famous scientist at Bell Labs in optical communications, believed that the transmitter rate was increasing from 100Gb/s to 200-400Gb/s based on the development of optical network capacity before 2018, by 2027 there will be 1000-1100Gb/s, and by 2037 there will be 2000-6000Gb/s[5]. Therefore, for an optical modulator, as the key device, its modulation bandwidth will reach 100GHz or higher.
In this work, we chose a barium titanate (BaTiO₃) crystal thin film with the ultrahigh electro-optic (EO) effects because its ultra-high EO coefficient is one of the choices for the next generation of EO modulation technology with its high potential in the applicable device development. In order to obtain accurate bandwidth goal of BaTiO₃ crystal thin film waveguide modulator, the accurate measurements of EO characteristics are very important. In 2013, Abel and others published BaTiO₃ crystal film EO coefficient test method[6], in 2019 they improved the testing methods, make the EO coefficient $r_{51}$ test precision is up to $\pm23\%$[7], then using a Mach-Zehnder interferometer (MZI) EO modulator structure, obtained the excellent performance of BaTiO₃ crystal thin film modulator beyond the state-of-the-art silicon-based devices, such as $V_{\pi L}$ and $V_{\pi L\alpha}$[8]. In 2015, Castera et al. studied the EO characteristics of BaTiO₃ and derived a theoretical model of quasi-linear EO modulation[9].
2. Theoretical Model and Experimental Strategy of Electro-optic Modulations

2.1. The Theoretical Model for the Measurements of Electro-optic Coefficient and Birefringence

Figure 1 shows an embedded configuration of BaTiO$_3$ crystal film waveguide EO modulation. In this configuration, BaTiO$_3$ crystal film is grown on magnesium oxide (MgO) crystal, the device parameters are defined as: $t_m$, $W_m$ and $G_x$ are the thickness, width and gap of the electrodes, respectively, $W_r$ and $H_r$ are the waveguide width and height, respectively, $T_f$ is the thickness of BaTiO$_3$ crystal thin film, $S_z$ is the embedded depth. In our previous work, with the embedded device configuration, a two-dimensional (2D) interaction between the optic field and the electric field can be realized and then the usual maximum 65% overlap integral of the traditional co-planar waveguide (CPW) regime based one-dimensional (1D) can be improved to be over 85% in numerical calculations$^{[10]}$. However, in the fabrication process, the uncertainty of the optic-electric interaction efficiency can also cause the influence on the measurement accuracies based on the measurement method in this work.

![Theoretical model of EO modulation](image)

**Figure 1.** The theoretical model of EO modulation.

As shown in Figure 1, an optical phase modulator structure uses the waveguide/electrode embedded configuration. If a drive voltage $V_g$ is imposed onto the waveguide through the pair of electrodes: anode and cathode, an electric field $E_d$ is created within the optical field $E_{opt}$, and then the interaction efficiency $\Gamma_{2D}$ between the $E_{opt}$ and $E_d$ is defined by an overlap integral formula as$^{[10]}

$$
\Gamma_{2D} = \frac{G}{V_g} \frac{\int\int E_d(x,z) E_{opt}(x,z) \, dx \, dz}{\int\int |E_{opt}(x,z)|^2 \, dx \, dz}
$$


**Figure 2.** Simulation results of the optic-electric interaction efficiency for the given embedded device structure with respect to three values of electrode gap.
In this work, we design and fabricate an experimental device sample, in which the device parameters $t_m$, $W_m$, $G_x$, $W_r$, $H_r$, $T_f$ and $S_z$ are designed to be 1$\mu$m, 40$\mu$m, 10$\mu$m, 4$\mu$m, 0.1$\mu$m, 0.5$\mu$m and 0.1$\mu$m, respectively. In addition, the length of electrode and the thickness of MgO substrate are 3.6mm and 500$\mu$m, respectively. Then, with the software - BPM we can obtain the optical field distribution of the guided mode and with the software - Quick Field we can obtain the electric field distribution. Then, by setting three gap values as 6$\mu$m, 8$\mu$m and 10$\mu$m, with equation (1), we obtain the interaction efficiency between the optic field and electric field with the embedded depth $S_z$ as shown in Figure 2. Note that the function $\Gamma_{2D}$ is a quasi-linear function when it is larger than 0.06$\mu$m irrespective of the electrode gap value. In addition, the smaller the electrode gap, the higher the tangential value of the linear function is, but the three lines intersect one another at the value of $S_z=0.16 \mu m$.

2.2. Experiments of Polarization Modulation

Figure 3(a) shows an experimental setup for the experiments of EO modulation and Figure 3(b) is the photo of a device sample of BaTiO$_3$ crystal film EO modulation structure as the device under testing (DUT). What needs to be clarified about the DUT is that the BaTiO$_3$ crystal film is directly taken as the c-axis oriented based on the testing results of the crystalline orientation of BaTiO$_3$ crystal films in previous work that used the same film growth technique - pulse laser deposition (PLD) as used in this work\cite{11}. Therefore, the electrodes are designed to create an electric field at the a-axis direction in plane of film. An optical beam at 1550nm wavelength from the light source goes through a polarizer to produces linear polarization state before it is launched into the waveguide, and PA is a polarization analyser used to detect modulated optical signals. With the experimental setup shown in Figure 3(a), we plan to carry out three refractive index modulations by imposing three values of the drive voltage to the BaTiO$_3$ crystal film waveguide in the device sample as shown in Figure 3(b).

![Experimental facility for polarization modulation: (a) is the experimental setup and (b) is the device sample for the polarization modulation where an electric field is applied at the a-axis direction.](image)

**Figure 3.** Experimental facility for polarization modulation: (a) is the experimental setup and (b) is the device sample for the polarization modulation where an electric field is applied at the a-axis direction.

![Experiments of the polarization characteristics of the output under several drive voltages.](image)

**Figure 4.** Experiments of the polarization characteristics of the output under several drive voltages. All the polarization states under the refractive index modulation are shown in Figure 4. With the polarizer and the polarization analyser (PA) shown in Figure 3(a) we set the input polarization state of an optical beam to be a left 45$^\circ$ linear state as shown in Figure 4(a), then launch it into a waveguide of the DUT that has a length of 6.0mm, the output guided mode has an initial output polarization state of the left 45$^\circ$ ellipse as shown in Figure 4(b). We perform the three continuous critical linear polarization states as the left 45$^\circ$, the right 45$^\circ$ and the left 45$^\circ$ under three values of drive voltage as shown in Figure 4(c), 4(d) and 4(e), respectively. Note that the first critical linear polarization state is
the same as the input state. So, we set \( V_d(m) \) \((m=2, 3 \text{ and } 4)\) and carry out two times of the above experiments and all the polarization states and the drive voltage values applied are summarized table 1.

Table 1. The \( V_d(m) \) values of linear polarization modulations.

| Modulation Processes & Drive Voltage Values | The 1\(^{st}\) switching | The 2\(^{nd}\) switching | The 3\(^{rd}\) switching |
|---------------------------------------------|--------------------------|--------------------------|--------------------------|
| \( V_d(2), V_d(3), V_d(4) \)               | 4.5V                     | 5.2V                     | 7.7V                     |
| \( V_d(2), V_d(3), V_d(4) \)               | 4.4V                     | 5.0V                     | 7.5V                     |

As a result, if there is an activation electric field existing in the crystal domains, we set an activating voltage to overcome it and then have the relation between the drive voltage \( V_d(m) \) value and the \( m \) value for the \( m' \)th linear polarization modulation as defined by equation (2) as

\[
r_{51} = \left( \frac{m \lambda}{L} \cdot \frac{1}{n_o^2 + n_e^2} \right)^{1/2} \cdot \frac{G_e}{[V_d(m) - V_{acr} \cdot \Gamma_{2D}]} \]  

(2)

where the birefringence of the crystal film under the EO modulation state is defined as \( b_{eo} = n_e - n_o \), and in this work we will carry out three optical phase modulations as \( m=2, 3 \) and 4.

2.3. The Theoretical Model for the Measurement Accuracies of Electro-optic Effect and Birefringence

It can be found from the equations (1) and (2), in the theoretical model for the measurements of EO coefficients and birefringence, \( V_d(m) \) and \( \Gamma_{2D} \) are changeable. So, the measurement accuracies are dependent of these two changeable parameters. By setting three different EO polarization modulations, we can obtain the measurement values of the coherent \( r_{51} \) and \( b_{eo} \) of BaTiO\(_3\) crystal film for the linear polarization states and further repeat multiple experiments of the modulations of the polarization state to obtain the average values of \( r_{51} \) and \( b_{eo} \). In fact, any effective measurement method for the key physical parameters must experience the errors that are probably caused by the principle of measurement method and the experimental operations. So, it is necessary to analyse the intrinsic measurement accuracies determined by these two elements.

In the experiments, the PA has an average polarization degree of 99.91\% for all the linear polarization states, so we neglect the influence of polarization degree on the measurement errors of BaTiO\(_3\) crystal film waveguide modulator, and instead only consider the effects of the controllable accuracy of the drive voltage \( V_d(m) \) and the fabrication/calculation accuracy of the optic-electric field interaction efficiency \( \Gamma_{2D} \) in the below context. Since the e-light has the refractive index of \( n_e = n_o + b_{eo} \), we operate the partial derivatives to equation (2) for the function \( r_{51} \) and \( b_{eo} \) with respect to variables \( V_d(m) \) and \( \Gamma_{2D} \), and then obtain equation (3) as

\[
\frac{n_e^2}{b_{eo}} r_{51} db_{eo} - 2 n_e^3 r_{51} db_{eo} + 4 r_{51} db_{eo} = -\frac{m \lambda}{L} \left[ \frac{G_e}{\Gamma_{2D}} \right]^2 \left( \frac{1}{V_d(m)} \right) dV + \left( \frac{G_e}{V_d(m)} \right)^2 \left( \frac{1}{\Gamma_{2D}} \right) d\Gamma 
\]  

(3)

Further, after considering the initial birefringence difference \( B_{eo} \) of the BaTiO\(_3\) crystal film waveguide, for the two modulation states of \( 2\pi \) and \( 3\pi \) optical phases under \( V_d(2) \) and \( V_d(3) \), respectively, \( B_{eo} \) should have the different values for the two modulations of \( 2\pi \) and \( 3\pi \) optical phases. So, we have two relations between the derivatives of \( r_{51} \) and \( b_{eo} \). Hence, for the optical phase modulations of \( 2\pi \) and \( 3\pi \), by introducing the influence of the initial birefringence \( B_{eo} \), we change equation (3) to (4) as
\[ n_3^2 \left\{ \frac{n_r r_{51}}{2(b_{eo} + C_{eo}(m)B_{eo})} - \left( \frac{n_r}{b_{eo} + C_{eo}(m)B_{eo}} + 4 \right) \right\} dr_{51} = \frac{m\lambda}{L} \left[ \frac{G_s}{r_{51} \Gamma_{2D} V_d(m)} \right]^2 \left( \frac{dV}{V_d(m)} + \frac{d\Gamma}{\Gamma_{2D}} \right) \]  

(4)

where \( m = 2 \) and 3, \( C_{eo}(2) \) and \( C_{eo}(3) \) stand for the corresponding effective impacting factors of the initial birefringence \( B_{eo} \) in the polarization EO modulation process.

3. Simulations for the Measurement Results of \( r_{51} \) and \( b_{eo} \), and the Measurement Accuracies

3.1. Simulations for the Measurement Results of EO Coefficient and Birefringence

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure5.png}
\caption{Simulations for the \( r_{51} - b_{eo} \) relations in the EO modulation process of BaTiO_3 thin film waveguide where (a) and (b) are from the two sets of polarization modulations depicted in table 1.}
\end{figure}

In accordance with the research of Towner et al. in 2004, \( n_o = 2.39, n_e = 2.37 \)\(^{[12]}\), we obtain the initial birefringence \( b_{eo} = -0.02 \). In fact, the effect of \( b_{eo} \) is not only dependent of its amplitude, but also the relative angle between the initial and the modulated polarization states. So, in computing the solutions with the experimental results listed in table 1, its value taken does not affect the solutions of \( r_{51} \) and \( b_{eo} \). With the two sets of experimental values listed in table 1 and equation (4), for the first and second sets of data in table 1, by setting the activation voltages of \(-3.3V\) and \(-3.1V\), we obtain the three \( r_{51} - b_{eo} \) relations as shown in Figure 5(a) and Figure 5(b), respectively. Then, it can be found that in each of the two figures, only one intersection point is formed because the two lines of \( 2\pi \) and \( 4\pi \) modulations are completely overlapped. Consequently, in Figure 5(a) and Figure 5(b), the coordinates of this intersection point are obtained to be \( b_{eo} = -0.0142/ r_{51} = 572pm/V \) and \( b_{eo} = -0.0127/ r_{51} = 567pm/V \), respectively, which can be taken as the final measured values of \( r_{51} \) and \( b_{eo} \) leading to the average values as \( b_{eo} = -0.0135 \) and \( r_{51} = 570pm/V \). Further, as the measurement accuracy, we obtain the standard deviation (SD) as \( \pm 2pm/V \) and \( \pm 0.0007 \) for \( r_{51} \) and \( b_{eo} \), respectively.

3.2. Simulations for the Dependences of Relative Measurement Error on Drive Voltage

It can be noticed from equation (4) that the deviation of the drive voltage \( dV/V_d \) and the deviation of the optic-electric interaction efficiency \( d\Gamma/\Gamma_{2D} \) have the same position, so only simulate the influences of \( dV/V_d \) on \( dr_{51}/r_{51} \) and \( db_{eo}/b_{eo} \) at first. We select one set of measured results as \( r_{51} = 567 \) pm/V and \( b_{eo} = -0.0127 \) to simulate the dependences of the measurement errors on the deviation of the drive voltage. In equation (4), by taking \( m = 2 \) and 3 to obtain two equations of the optical phase modulation, and then combing these two equations to obtain two independent equations of \( dr_{51}/r_{51} \) and \( db_{eo}/b_{eo} \) with respect to \( dV/V_d \), and further carry out the numerical simulations of
$dr_{51}/r_{51}$ and $db_{eo}/b_{eo}$ as shown in Figure 6(a) where the blue and green lines stand for $dr_{51}/r_{51}$ and $db_{eo}/b_{eo}$, respectively. Note that the $dr_{51}/r_{51}$ has much more dependence on $dV/V_d$ than the $db_{eo}/b_{eo}$. Accordingly, hereafter we only study the dependence of one relative accuracy, $dr_{51}/r_{51}$, the key variable in the measurements.

With equation (4) we obtain the numerical simulation results for the relation between $dr_{51}/r_{51}$ and $dV/V_d$ with respect to the optical phase modulations as shown in Figure 6(b) where the blue and green lines stand for the EO modulations of $2\pi$ and $3\pi$ optical phases, respectively.

**Figure 6.** Measurement accuracy analysis for the results of $r_{51}$ and $b_{eo}$ with the linear polarization modulation: (a) is the dependences of $r_{51}$ and $b_{eo}$ on $dV/V_d$ and (b) is the measurement accuracy dependences of $r_{51}$ on $dV/V_d$ at $2\pi$ and $3\pi$ optical phase modulations.

From Figure 6(b), it can be found that the errors of the first voltage for $2\pi$ optical phase modulation and the second voltage for the $3\pi$ optical phase modulation have the very similar influences on $dr_{51}/r_{51}$, but $dV/V_d$ for these two optical phase modulations has the stronger influences on $dr_{51}/r_{51}$ at the first modulation than the second one. For instance, at the $2\pi$ optical phase modulation, when the accuracy of $dV$ reaches 1.0%, the measurement value of $r_{51}$ is lower than the real value by 7.0%, while for the $3\pi$ optical phase modulation, the measurement value of $r_{51}$ is lower than the real value 5.0%.

Accordingly, we conclude that if the relative accuracy of $V_d$ value is controlled to be $\pm1.0\%$, the relative accuracy of $r_{51}$ can be controlled under $\pm5.0\%$. The consequent conclusion for the experiments of linear polarization characterizations is that, for the $2\pi$ optical phase modulation, the drive voltage is 4.4V, so the accuracy of $\pm1.0\%$ for $V_d$ means an absolute error under $\pm0.04V$.

**4. Conclusion**

The correct determination of the axis orientation and the accurate measured values of the key physical parameters of BaTiO$_3$ crystal film are very sustainable to developing a waveguide EO modulator from a laboratory sample to an industrial product. Specially, an ultrahigh bandwidth EO modulator, the highly accurate measurement for the central parameter such as the EO coefficient is a crucial condition to develop the high-performance EO modulators and other functional devices with an efficient use of the advancements of tetragonal crystal material. Well aware, the supper accurate measurements of $r_{51}$ and $b_{eo}$ of a BaTiO$_3$ crystal film in this work will provide the reliable data to the research and development of EO modulation devices. Illustratively, for the ferroelectric crystal waveguide modulator, EO coefficient plays a crucial effect in the figure of merit (FOM), further determines the optic-electric interaction length that is the key factor in determining the potential bandwidth of an EO modulator. The other important finding is that the optic-electric interaction efficiency and drive...
voltage accuracy have the simultaneous influences on the measurement accuracy of $r_{51}$. Thus, it turns out that the theoretical study and analysis for the relative measurement accuracies of $r_{51}$ and $b_{eo}$ are conducive to research and development of the BaTiO$_3$ crystal film based EO modulation devices.

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