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Electro-Optical Modulation based on Pockels effect in $BaTiO_3$ with a Multi-Domain Structure

Pau Castera, Ana M. Gutierrez, Domenico Tulli, Sébastien Cueff, Regis Orobtchouk, Pedro Rojo Romeo, Guillaume Saint-Girons, and Pablo Sanchis

***Abstract*— The influence of an in-plane multi-domain structure in $BaTiO_3$ films grown on $SrTiO_3$/Si buffers for highly efficient electro-optic modulation has been analyzed. The modulation performance can be significantly enhanced by rotating a certain angle the optical waveguide with respect to the $BaTiO_3$ crystallographic axes. A robust electro-optical performance against variations in the domain structure as well as the lowest V_π voltage can be achieved by using rotation angles between 35º and 55º. Our calculations show that V_π voltages below 1.7 V for a modulation length of 2 mm can be obtained by means of a CMOS compatible hybrid silicon/$BaTiO_3$ waveguide structure.**

***Index Terms*—Waveguide modulator, modulators, electro-optical devices, ferroelectrics.**

I. INTRODUCTION

Integration of complex optical functionalities with high performance is leading to a huge development in the field of nanophotonics for a broad range of applications. Photonics technology based on silicon-on-insulator (SOI) allows compatibility with CMOS fabrication processes. This makes the silicon platform as one of the best candidates to implement mass-manufacturable low-cost nanophotonic devices. However, the centrosymmetric nature of silicon prevents its use for enabling electro-optical (EO) modulation based on the Pockels effect. Several approaches have been pursued to overcome such limitation. So far, the most used mechanism to modulate the refractive index in silicon is the plasma dispersion effect, which consists in varying the free-carrier concentration in doped silicon. Unfortunately, one of the main issues is that there is a trade-off between low insertion losses and low driving voltage [1].

EO modulation via the Pockels effect allows achieving high modulation efficiency at very fast speed without penalizing insertion losses. By breaking the crystal symmetry of silicon, Pockels effect has been confirmed [2] and promising results have been accomplished by using highly stressing layers on top of the silicon waveguide [3]. Nevertheless, recent studies have shown that free carriers have a prominent role and one order of magnitude lower effective Pockels coefficient has been measured at high frequencies [4]. On the other hand, ferroelectric oxides, and in particular barium titanate ($BaTiO_3$ or BTO), have been proposed for developing highly efficient EO modulators because of their high Pockels coefficients [5]. In its bulk form, BTO exhibits a much larger Pockels coefficients than that of $LiNbO_3$, the reference EO material. Integrated photonic devices based on BTO have been broadly investigated on magnesium oxide substrates [6–10]. However, the possibility for growing high quality BTO thin layers on SOI substrates using $SrTiO_3$ buffers has opened a path towards the development of EO modulators with disruptive performance [11-15].

In our previous work [16], the optimum BTO ferroelectric domain orientation to enhance the EO modulation was analyzed assuming a single domain orientation, achieving a $V_\pi \cdot L_\pi$ as low as 0.27 V·cm. However, a multi-domain structure is usually formed during the fabrication of $BaTiO_3$ layers [17, 18]. In the present work, we carefully investigate the influence of the multi-domain structure, as well as the waveguide rotation angle, on the EO modulation performance.

II. THEORETICAL BACKGROUND

BTO is a ferroelectric material with perovskite crystal structure. Above Curie temperature (T_C=120ºC for BTO), this material has a centrosymmetric cubic structure and thus behaves like a dielectric without spontaneous polarization. On the contrary, below Curie temperature (at room temperature) its crystal structure changes to tetragonal phase thus yielding to a stretching of the '*c*' lattice parameter and a corresponding shrinking of '*a*' and '*b*' parameters (*a*=*b*). In this situation, the material is non-centrosymmetric and presents a spontaneous polarization parallel to the crystallographic c-axis.

The EO performance will depend on how the BTO is grown before the fabrication of the waveguide structure. Specifically, the tetragonal form of the crystal structure implies that the

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material can be grown with two different orientations depending on the process conditions: an in-plane polarization of tetragonal BTO films implies that the *c*-axis is along the growth plane (usually defined as *a*-axis orientation). Oppositely, an out-of-plane polarization indicates a BTO film with its *c*-axis perpendicular to the growth plane (usually defined as *c*-axis orientation). Furthermore, the resulting orientation of BTO film can vary from purely *a*-axis to *c*-axis orientations, through a mixture of *a* and *c*-axes oriented configurations [17]. Epitaxial growth of BTO films offers the possibility to select the direction in which the spontaneous polarization can appear depending on the desired application [18]. In this work, we will consider purely *a*-axis oriented BTO films as it has been shown to provide better EO performance [15, 16].

III. RESULTS AND DISCUSSION

The proposed hybrid silicon/$BaTiO_3$ waveguide structure for enabling EO modulation is shown in Fig. 1(a). An amorphous silicon (a-Si) layer is deposited on top of the previously grown BTO and then etched to form a slot waveguide which provides high optical confinement. Furthermore, aluminum electrodes are placed directly on top of the BTO in order to obtain a stronger electric field in the active region. Finally, the waveguide structure is covered by a SiO_2 cladding.

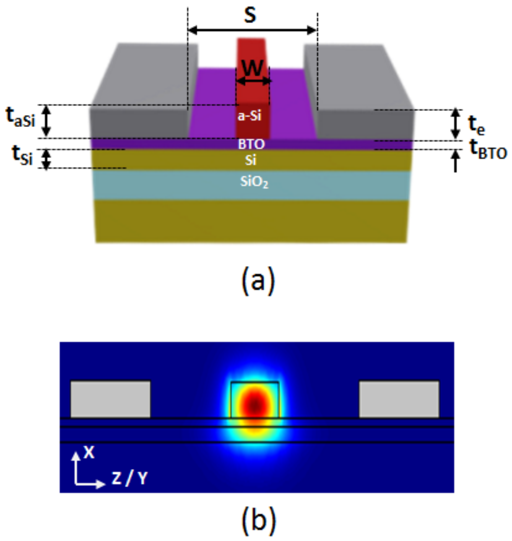

Fig. 1. (a) Schematic of the waveguide cross-section and (b) fundamental mode profile for TE polarization at a wavelength of 1.55 µm.

The waveguide parameters, which are also depicted in Fig.1(a), have been optimized by simulations [16]. The thickness of the silicon layer in the SOI wafer is t_{Si}=100 nm and the BTO thickness is t_{BTO}=50 nm. The rest of the parameters have been selected to achieve simultaneously single-mode operation with negligible losses and high optical confinement in the BTO layer. Therewith, we have obtained an a-Si thickness of $t_{a\text{-}Si}$=220 nm, a waveguide width of W=600 nm and a separation between electrodes of S=2 µm for TE polarization. The separation between electrodes has been chosen to keep the optical losses induced by the metal electrodes below 1dB/cm. The fundamental mode profile is shown in Fig. 1(b) at a wavelength of 1.55 µm.

BTO, as a negative uniaxial anisotropic crystal, presents an ordinary refractive index (n_o=2.444) larger than its extraordinary index (n_e=2.383) [15]. The EO performance can be modeled by means of the index ellipsoid equation, which in the case of a single-domain BTO film and TE polarization is reduced to the following ellipse equation

$$\left(\frac{1}{n_o^2}+r_{13}E_z\right)y^2+\left(\frac{1}{n_e^2}+r_{33}E_z\right)z^2+\left(r_{51}E_y\right)2yz=1 \quad (1)$$

where r_{ij} are the linear (or Pockels) EO coefficients and (E_z, E_y) are the applied electric field components. It is assumed that the out-of-plane component of the applied electric field is negligible ($E_x \approx 0$) due to the electrodes configuration. The considered values for the electro-optic tensor components are r_{13}=8 pm/V, r_{33}=28 pm/V and r_{42}=r_{51}=800 pm/V [16]. In the case of a single domain BTO film, two extreme cases can be initially considered: when the electric field is parallel (E_y=0) or when it is perpendicular (E_z=0) to the optical BTO axis. In the former only the r_{13} coefficient is involved while in the latter there is no modulation. Nevertheless, the EO performance can be significantly enhanced by rotating a certain angle the waveguide with respect to the BTO crystallographic axes thus achieving an EO coefficient that will be a linear combination of r_{13}, r_{33} and r_{51}.

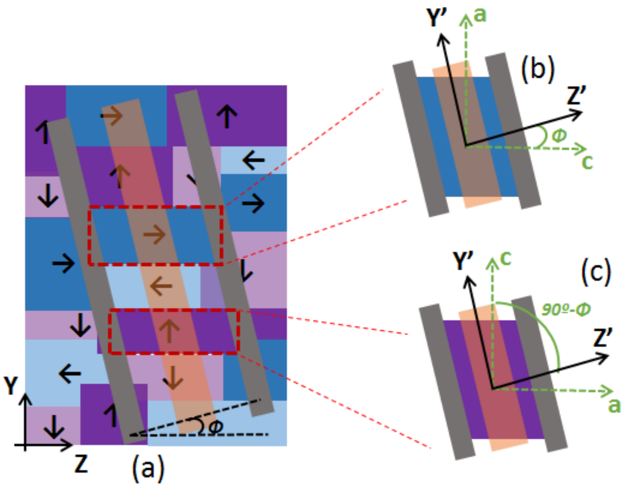

Fig. 2. (a) Top view schematic of the optical waveguide with electrodes rotated by a certain angle, ϕ , which is defined with respect to the z-axis. The influence of the multi-domain BTO structure is analyzed by separately considering (b) 0° and (c) 90° domains. The arrow indicates the spontaneous polarization present in the tetragonal form of BTO which is parallel to its crystallographic c-axis.

Figure 2(a) shows a top view of the rotated waveguide with the rotation angle, ϕ, defined with respect to the z-axis. Four in-plane domain variants, with their polarization directions represented by arrows, can be distinguished in *a*-axis oriented

BTO films [11]. It is assumed that domains along the optical waveguide do not change their orientation in the z direction and neither due to the presence of the applied electric field. In order to analyze the influence of the multi-domain BTO structure, the so-called 0º domains (see Fig. 2(b)) and 90º domains (see Fig. 2(c)) must be separately considered.

Focusing on 0º domains and initially considering that there are not antiparallel domains along the optical waveguide, the index ellipsoid when the waveguide is rotated can be obtained by applying a transformation from the original *zy* coordinate system to a new *z'y'* coordinate system, which is defined along the applied electric field and the propagation of light [16]. Thereby, the EO coefficient and BTO refractive index can be derived for TE polarization as:

$$r_{z'}(\phi) = r_{33}\cos^3(\phi) + (r_{13} + 2r_{51})\sin^2(\phi)\cos(\phi) \quad (2)$$

$$n_{z'}(\phi) = \frac{n_o n_e}{\sqrt{n_e^2 \sin^2(\phi) + n_o^2 \cos^2(\phi)}} \quad (3)$$

From Eq. (2), the EO coefficient assuming a randomly mixed BTO domain distribution can be modelled by the following equation:

$$r_{eff}(\phi,\alpha) = r_{z'}(\phi) + \alpha[r_{z'}(90^{\circ} - \phi) - r_{z'}(\phi)] \quad (4)$$

where α is related to the orientation of the domains, taking values between 0 (all domains 0º oriented) and 1 (all domains 90º oriented). A similar expression can be derived from Eq. (3) to calculate the BTO refractive index, $n(\phi,\alpha)$, in the presence of mixed domains.

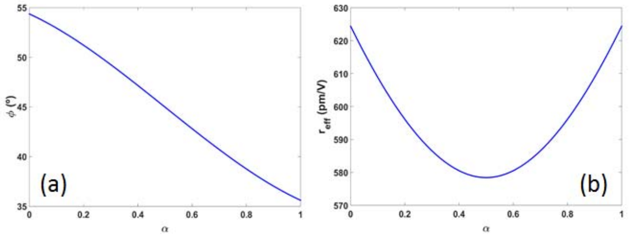

Fig. 3. (a) Optimum rotation angle to have (b) the highest Pockels coefficient depending on the mixed BTO domain distribution (α parameter).

The presence of a multi-domain structure will give rise to an optimum rotation angle of the optical waveguide to have the highest effective Pockels response depending on the α parameter. Figure 3 shows the obtained results. The optimum angle shifts from 35º for α=1 to 55º for α=0, obtaining the highest value of r_{eff}=624 pm/V in both cases. Furthermore, for equally-mixed domain variants, i.e. for 50% of 0º and 90º domains (α=0.5), a local minimum can be seen in Fig. 3(b), but the effective Pockels coefficient remains high (r_{eff}=578 pm/V).

The refractive index and EO coefficient have been used to analyze the influence of the multi-domain structure on the V_π voltage of the modulator for different rotation angles of the optical waveguide. In a Mach-Zehnder modulator, the V_π voltage can be analytically estimated by using a first order approximation as:

$$V_{\pi,TE}(\phi,\alpha) \approx \frac{\lambda S}{\Gamma_{TE} n^3(\phi,\alpha) r_{eff}(\phi,\alpha) L} \quad (5)$$

where λ is the wavelength, S is the separation between the electrodes, L is the active length and Γ_{TE} is the EO overlap integral for TE polarization. In our case, the active length has been fixed to L=2mm, λ=1550nm, S=2μm and Γ_{TE}=11.66%.

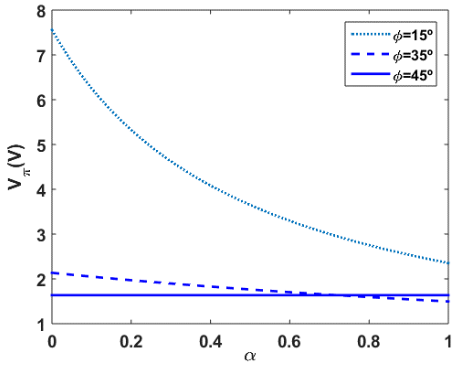

Fig. 4. V_π voltage as a function of the α parameter for three different rotation angles of the optical waveguide.

Figure 4 shows the V_π voltage as a function of the α parameter for three different rotation angles. It can be seen that the lowest V_π voltage (below 1.5 V) is achieved for the optimum rotation angle of ϕ=35º, which provides the highest Pockels coefficient but only when most of the domains are 90º oriented (α≈1). However, the V_π voltage increases when more 0º domains are present. On the contrary, it is interesting to notice that for a rotation angle of ϕ=45º, the V_π voltage has a constant value of 1.64 V and it does not depend on the α parameter and therefore on the in-plane domain structure. This behavior can be easily proved by looking at Eq. (4) and implies that a higher robustness in the EO performance will be achieved at the expense of a small penalty on the V_π voltage due to a slightly smaller effective Pockels coefficient. On the other hand, when the rotation angle is far away from 45º, there is a large dependence of the V_π voltage with respect to the multi-domain structure, as it can be clearly seen in Fig. 4 for ϕ=15º.

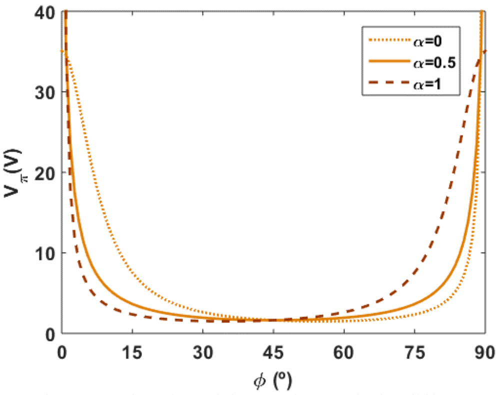

Fig. 5. V_π voltage as a function of the rotation angle for different BTO domain distributions (α parameter).

Figure 5 shows the V_π voltage as a function of the rotation angle of the optical waveguide for different BTO domain distributions. The lowest V_π voltage for α=0 (0º domains) is found at rotation angles above 45º while for α=1 (90º domains) it is obtained at rotation angles below 45º. However, it can be seen that these low V_π voltages will drastically increase for rotation angles below 15º or above 75º. Furthermore, it can also be clearly observed that the dependence of the V_π voltage with the BTO domain distribution significantly increases when the rotation angle is not close to 45º, as it was also shown in Fig. 4.

Results shown in Figs. 3, 4 and 5 have been obtained considering that antiparallel domains are not present independently of the α parameter. However, it can be deduced from Eq. (2) that the EO coefficient will have a different sign in antiparallel domains. Therefore, the phase shift accumulated by the optical mode will be canceled when travelling through antiparallel domains (see Fig. 2(a)). This effect can be simply modelled as a reduction of the effective active length. From Eq. (5), a lower active length will be proportional to an increase of the V_π voltage. In the proposed modulator, a percentage of antiparallel domains as high as 66% of the total number of domains present across the active length can be supported to keep the V_π voltage below 5V.

IV. CONCLUSION

The influence of an in-plane multi-domain structure on the EO modulation performance has been analyzed. Results have been obtained for a silicon CMOS compatible structure but the main findings can be generalized for any kind of optical waveguide structure. It has been shown that the placement of the optical waveguide with respect to the orientation of BTO domains is critical. More concretely, the lowest V_π voltage is achieved by rotating the optical waveguide with an angle between 35º and 55º depending on the multi-domain structure. The most robust angle against variations in the domain structure is 45º but at the expense of a slightly higher V_π voltage.

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