Low Driving Voltage Lithium Niobate Metasurface

² Electro-Optical Modulator Operating in Free

Space

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Abstract: A simple configuration of only $\lambda/9$ thick 2D metallic grating embedded within an 8 electro-optic (EO) material (lithium niobate for instance) is proposed and theoretically studied 9 to act as an EO modulator. On the first hand, this grating is used as an interdigitated comb to 10 apply a very high and spatially periodic modification of the electrostatic field. On the other 11 hand, the grating is designed to exhibit a Fano-like resonance in the NIR spectral range. This 12 resonance is used to confine the electromagnetic field inside the EO material leading to an 13 intrinsic enhancement of the EO effect. Extensive numerical simulations are performed to 14 optimize the geometry in agreement with technological fabrication constraints. We achieved a 15 local field factor of 24.5 leading to a local index modification Δn as large as 1 for 1 V applied 16 voltage. This allows a modulation sensitivity of 14.35 nm/V (2000 times larger than the state of 17 the art) together with a resonance depth= of 60% and a driving voltage of only 75 mV opening 18 the way to the fabrication of ultra-thin low driving voltage EO devices. 19

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21 1. Introduction

Electro-optical (EO) modulators required to convert electrical signals into optical informations 22 are crucial and in very high demand for most optical-based devices and telecommunication 23 systems [1, 2]. In this context, lithium niobate (LiNbO₃) is known as one of the best candidate for 24 EO devices due to its important physical properties, notably its high EO coefficients [3–5]. It offers 25 a wide transparency band, which opens the range to applications from visible to mid-infrared. 26 The dominance of LiNbO₃ in EO technologies is related to its higher Curie temperature compared 27 to other EO materials, which makes it robust to temperature variation and harsh environments. 28 The efficiency of an EO modulator is linked to the electric voltage needed to drive the modulator 29 and to the footprint of the device that can be assessed with the $V_d \cdot L$ figure of merit, where V_d 30 is the driving voltage and L the active length. In general, commercial EO modulators made of 31 LiNbO₃ and based on a Mach-Zehnder interferometer (MZI) present a half wave voltage between 32 3 V [6] and 1 V [7] with an active length larger than one centimeter. 33

After the emergence of thin-film lithium niobate (TFLN) [8,9], a new era in photonics 34 technology has begun, leading to EO devices with reduced footprint and driving voltage. In 35 the last couple of years, the progress remains improving in order to conceive EO modulators 36 with lower half wave voltage (V_{π}) and larger bandwidth taking advantage of TFLN [10–12]. 37 In [10], they achieved a 1 V driving voltage and 110 GHz bandwidth in a TFLN-modulator 38 that works in dual-polarization, enabling a record single-wavelength 1.96 Tb/s net data rate. 39 However, Weiss et al. [12] proposed a plasmonic nanoscale metasurface array coupled with a 40 TFLN and reach a wavelength tunablity of 3 nm for a 50 V peak-to-peak voltage difference. 41 Generally, the voltage-length product $(V_{\pi} \cdot L)$ of the TFLN modulator is 1.5 to 3 V·cm [13, 14], 42 which is considerably lower than that of commercial LN modulators (15 V \cdot cm) [1] at telecom 43 wavelengths. 44

Photonic Crystals (PhC) can exalt EO interactions and gain even more than an order of magnitude on the figure of merit compared to MZ-based architectures [15]. Moreover, PhC architecture can thereby shrink down the device footprint which reduces its capacitance and the required switching voltage. The emergence of PhC-based devices has increased the integration of photonic devices to meet the requirements of embedded technologies and become competitive with electronic devices.

A LiNbO₃ PhC modulator was proposed since 2007 to enhance the EO effect by locally 51 confining the electromagnetic field when a Bloch mode is excited within the PhC [16]. This 52 becomes relevant when the group velocity of this Bloch mode is very small. In this case, the time 53 interaction between light and matter grows significantly leading to exacerbate all the intrinsic 54 non-linear coefficients of the considered material, among others, the second order susceptibility 55 term $\chi^{(2)}$ involved in the EO effect. Such enhancement was experimentally [17] verified 56 and theoretically explained. Thereby, a new generation of EO modulators [18], pyroelectric 57 detectors [19] or Second Harmonic Generation (SHG) devices [20] were proposed, fabricated and 58 characterized validating the principle of this enhancement. Meanwhile, dark Fano resonances, 59 also know by optical bound state in the continuum (BIC), were also explored in order to exacerbate 60 the EO effect [21]. It provides an excellent electromagnetic field confinement essential to enhance 61 the EO effect surpassing a conventional guided resonance [22]. 62

Here, we proposed a simple Ag-LiNbO₃ configuration based on the excitation of a Fano-like resonance at $\lambda_{res} = 1530$ nm insuring the electromagnetic field confinement required to enhance the host medium EO coefficient. The geometry of the structure is inspired by the one studied in [23] where a miniaturized acousto-optic modulator based on sub-wavelength structures presenting simultaneously a photonic and phononic resonance has been proposed and studied demonstrating a strong optical modulation at near infrared wavelengths.

69 2. Proposed Structure

Unlike most common modulators, we propose a configuration operating in the Γ direction 70 (out-of-plane illumination at normal incidence), which allows us to illuminate the structure in 71 free space and overcome the optical losses that occur by an in-plane illumination such as the 72 injection losses and the propagation losses, as it is the case for MZI-based modulators. Our EO 73 modulator, as shown in Fig.1(a), is based on a simple configuration of a 2D metallic grating of 74 thickness $h = \lambda/9$, embedded in the LiNbO₃ in order to take advantage of the confinement of the 75 electromagnetic field induced by our Fano resonance. On one hand, this grating is used as an 76 interdigital comb to apply a very high and spatially periodic variation of the electrostatic field 77 leading to an enhancement of the EO effect and improvement of the EO sensitivity. On the other 78 hand, the grating is designed to optically exhibit a Fano type resonance in the NIR spectral range. 79 Our proposed structure relies on a 1D PhC structure with a grating lattice p. The unbalance 80 between the two LiNbO₃ cavities with two different widths W_1 and W_2 creates a mismatch 81 between the volume of the cavities and allow us to generate the well-known π -resonance also 82 known as phase-resonance. The origin of the optical resonance appearing on the transmission 83 spectrum through the structure has been discussed in [24]. In order to take advantage of the larger 84 EO coefficient of the LiNbO₃, the applied voltage and electromagnetic field must be oriented 85 parallel to the crystallographic Z-axis of the LiNbO₃, which requires an X- or Y-cut LiNbO₃ 86 slab. In the following, we will consider an X-cut LiNbO₃ structure and assume the LiNbO₃ 87 extraordinary refractive index $n_e = 2.2472$ to be constant in the spectral range of interest. 88 In order to adapt the geometry, extensive FDTD (Finite Difference Time Domain) simulations 89

with a custom code were performed to obtain resonance in the NIR spectral range with the highest Q-factor and the largest resonance depth (RD) corresponding to a maximum modulation amplitude. A uniform 2D mesh with a mesh size of $\Delta x = \Delta y = 2$ nm is applied to describe the structure. We consider an infinitely periodic structure in the *x* direction by applying the



Fig. 1. (a)Schematic of the proposed structure showing its geometrical parameters and (b) transmission spectra for TE polarization presented by blue circles and by solid red line for the TM-polarized incident plane waves. The geometrical parameters are: h = 170nm, p = 650nm, $W_1 = 150$ nm, $W_m = 120$ nm. The refractive index of LiNbO₃ is fixed to $n_e = 2.2472$ and the metal is silver.

Bloch periodic boundary conditions, and perfectly matched layer (PML) conditions are used 94 as absorbing boundary conditions to numerically truncate the substrate and superstrate media. 95 Approximately 1 million iterations are considered for a single calculation to achieve the stopping 96 criteria (steady states). All geometrical parameters were varied taking into account the fabrication 97 constraints (aspect ratio $AR = h/min(W_m, W_1, W_2)$ smaller than 2 and slit width larger than 98 80nm). The geometrical parameters of the optimized structure are: h = 170nm, p = 650 nm, 99 $W_1 = 150$ nm, $W_m = 120$ nm. Different metals were also studied (Ag, Al, Pt, Au) for the electrodes, 100 showing better results with silver. The latter presents the lowest optical absorption losses. Its 101 dielectric properties are adapted to [25] through a Drude critical points model [26]. 102 Fig.1(b) shows a typical transmission spectrum of light through the structure for the two 103 linear polarization states (TE and TM). As expected, the slit structure behaves as a metallic 104 grid polarizer with axis perpendicular to the slit direction. Consequently, only the Ox incident 105

¹⁰⁶ polarization can be transmitted. The resonance depth (RD) and the quality factor (Q-factor) are ¹⁰⁷ defined from this spectrum by: $RD = \frac{T_{\text{max}} - T_{\text{min}}}{T_{\text{max}}}$ and $Q = \frac{\lambda_{\text{res}}}{\Delta \lambda}$. Their values, respectively 77% ¹⁰⁸ and 318 for the resonance at $\lambda_{\text{res}} = 1529.6 \text{ nm}$, are above the experimentally required threshold ¹⁰⁹ values.

110 3. Results and Discussions

¹¹¹ In order to enhance the EO effect in LiNbO₃, the electric field must overlap with the optical mode ¹¹² in the LiNbO₃, in other words, the electric field and the electromagnetic field has to be confined ¹¹³ in the LiNbO₃ substrate leading to a dielectric mode and to the enhancement of the EO coefficient ¹¹⁴ r_{33} by a factor F_{opt} as described in equation 1, the expression of the local EO effect [16]:

$$\Delta n_{\rm e}(x,z) = -\frac{1}{2} n_{\rm e}^3 r_{33} F_{\rm opt}^2(x,z) E_{\rm es}(x,z), \tag{1}$$

where $F_{\text{opt}}(x, z)$ is the local optical field factor defined by

$$F_{\text{opt}}(x,z) = \frac{|\vec{E}(x,z)|_{\text{structure}}}{|\vec{E}|_{\text{bulk}}},$$
(2)

where $|\vec{E}|_{\text{bulk}}$ is the amplitude of the homogeneous E-field in the bulk LiNbO₃ substrate (without 116 PhC) and $|E(x,z)|_{\text{structure}}$ is the local amplitude of the E-field in the studied PhC structure. 117 To confirm the existence of a dielectric mode and then derive the optical field factor F_{opt} , we 118 calculate the electric field distribution at the resonance wavelength using a 2D-FDTD custom 119 code. As shown in Fig.2(a), the normalized electric field intensity reaches its maximum at the 120 corners of the electrodes and inside the LiNbO3 between the two electrodes leading to a dielectric 121 mode, which is consistent with the conditions required to enhance the EO effect. Based on the 122 optical field factor definition given in Eq.2, we reach a maximum of $F_{opt}^2(x, z) = 1100$, which 123 corresponds to a variation of the refractive index in the PhC structure up to 1100 times higher 124 than that of the bulk structure. The normalization has been established with the same FDTD 125 code and the same configuration of the calculation window without the nanostructure (periodic 126 metallic grid). However, as described in Eq.1, the EO sensitivity depends on $F_{opt}(x, z)$ and 127 electrostatic field distribution through $E_{es}(x, z)$. 128



Fig. 2. (a) Spatial distribution of the normalized electric field intensity (or $F_{opt}^2(x, z)$) at $\lambda_{res} = 1529.6$ nm. The white lines correspond to the structure edges. The zoom-in made over the highlighted rectangular zone on the left shows the electric field intensity to the power 0.4 to enhance the color contrast and presents clearly the electric field distribution in this zone. (b) Electrostatic field distribution (only the x-component) when a potential difference of 1V is applied between two consecutive electrodes.

After the estimation of F_{opt} distribution, we moved to the calculation of the electrostatic field distribution $E_{es}(x,z)$ in order to complete the missing values for the estimation of the EO effect of the proposed structure.

As previously explained, the applied electrostatic field $E_{es}(x,z)$ is polarized along the xdirections which corresponds to the crystallographic Z-axis for a X-cut LiNbO₃ wafer in order to benefit from the highest EO coefficient of LiNbO₃ (r_{33}). For this reason, we will only consider in our calculations the X-components of E_{es} since it will involve the highest EO coefficient of LiNbO₃ (r_{33}). Similarly, we will only focus on the electrostatic field confined inside the LiNbO₃ and not in the air, since the EO effect occurs only in the EO material (LiNbO₃ in our case). Indeed, no electrostatic field apart from the one in LiNbO₃ will contribute to the EO effect.

The same structure was modeled to solve the Poisson equation when a voltage of 1 V is applied between the two consecutive electrodes. Thus, COMSOL multiphysics software was used to this end by integrating periodic boundary conditions in the x-direction and Dirichlet boundary ¹⁴² conditions for the up and down limits of the calculation window. In addition, a very fine mesh, ¹⁴³ based on Delaunay triangulation, was applied in order to minimize the numerical errors when ¹⁴⁴ interpolating the $E_{es}(x,z)$ values over the regular square grid used in the FDTD simulations. The ¹⁴⁵ x-component of the electrostatic field presented in Fig.2(b) is showing a maximum value between ¹⁴⁶ the two electrodes and in the electrode corners immersed in LiNbO₃. It varies between 12×10^6 ¹⁴⁷ V/m and -8.2×10^6 V/m, values that are slightly larger than

$$\frac{V}{W_1} = \frac{1}{150 \times 10^{-9}} = 6.67 \times 10^6 \, V/m,\tag{3}$$

148 and

$$\frac{-V}{W_2} = \frac{-1}{260 \times 10^{-9}} = -3.85 \times 10^6 \, V/m,\tag{4}$$

respectively. This difference comes from the presence of electrode corners (90°) that induces an
enhancement of the electric field due to a well-known "antenna effect" that was widely studied
both theoretically [27,28] and experimentally [29,30].



Fig. 3. (a) Shift of the resonance induced by an applied voltage of 1 V (in red) and -1 V (in blue). In black, the transmission spectrum of structure before applying an electric voltage. Inset: the local refractive index distribution for 1 V applied voltage. (b) The evolution of the resonance wavelength with respect to the applied voltage. Inset in blue the transmission spectra of the structure for different electric voltage going from 0 V to 0.5 V with a step of 0.05 V and in black the transmission spectrum of the structure for 0 V.

To highlight the mechanism of modulation, we started by estimating the sensitivity of the structure as response of an applied voltage. To do so, we compute the electrostatic field distribution for an applied voltage of 1 V and -1 V using COMSOL and inject these values with the optical field factor distribution into Eq.1 in order to calculate the resonance shift by FDTD. In Fig.3(a), we present the calculated three transmission spectra pointing out the resonance shift induced by 1 V (in red) and -1 V (in blue) applied voltage. More details about the resonances are summarized in Table 1.

For just 1 V applied voltage, the resonance (in red) shift to 1515.293 nm with a Q-factor of 252 and a RD of 87.3%. However, with a -1 V applied voltage, the resonance (in bleu) shift to 1546.02 nm with a Q-factor of 135 and a RD of 92.4%. Despite the larger shift with a -1 V applied voltage, the decrease in the Q-factor of the resonance is directly linked to a lower optical field factor compared to the other resonance (with an applied voltage of 1 V). In the following,

Table 1. Details about resonances in Fig.3(a).

ΔV	$\lambda_{ m res}$	Q-Factor	RD	
0 V	1529.652 nm	318	77.3%	
1 V	1515.293 nm	252	87.3%	
-1 V	1546.02 nm	135	92.4%	

the modulation performance of the structure will be studied only with a positive applied voltage so we can benefit as much as possible from the EO enhancement of the proposed structure.

A sensitivity of 14.35 nm/V is estimated, which is 2000 times higher than the one recently achieved by Wang *et al.* [31]. The shift of the resonance wavelength with respect to the applied voltage is presented in Fig.3(b). Similarly, every point is computed by a couple of COMSOL-FDTD simulations. The trend of the curve with respect to the applied electric voltage is quasi-linear.

To end up with the modulation performance of the structure, we present in Fig.4 the optical 171 response of the structure with respect to the applied voltage. We considered a light detector 172 operating at the resonance wavelength, and we deduce the transmitted light for each applied 173 voltage. We clearly see that we reach a permanent state for an applied voltage V=0.2 V. This 174 means that our structure requires a driving voltage (V_d) as low as 0.2 V in order to go from the 175 ON to the OFF states. In order to improve the modulation of the structure, one can consider the 176 highlighted red zone where the transmission variation as function of the applied voltage is linear. 177 We conclude with a minimized driving voltage $V_d = 0.075$ V and an RD = 60% instead of $V_d =$ 178

 $_{179}$ 0.2 V and an RD = 80% if we consider the complete modulation zone presented in Fig.4.



Fig. 4. The optical response of the structure with respect to the applied voltage. Inset: the electric field amplitude at the ON and OFF state for V = 0 V and 0.2 V, respectively.

In order to be more realistic, we study the effect of a finite structure with a finite number of period on its optical response. For this purpose, 2D-FDTD simulations are performed to evaluate the normalized zero-order transmission spectra of the structure with a finite number of periods and the previously determined parameters. The Bloch periodic boundary condition are replaced by perfectly matched layer boundary conditions in order to simulate the finite structure with a uniform mesh size of $\Delta_x = \Delta_z = 10$ nm in the *x* and *z* directions instead of 2 nm in order to speed

- ¹⁸⁶ up our simulations. The larger mesh size considered in our simulations will induce a shift of the
- resonance wavelength according to [32]. The structure is illuminated by a Gaussian beam whose size is fixed at 100 μm .



Fig. 5. Normalized transmission with respect to the number of periods. The dashed green line indicates the resonance position for an infinitely periodic structure, while the dashed red line refers to the resonance position, for 50 periods, where the RD and the Q factor of the resonance become sufficient for modulation.

188

The 2D-FDTD simulations are conducted by varying the number of periods, going from 20 189 periods to 80 periods. The result is presented in details in Fig.5 and table 2. On one hand, 190 Fig.5 presents the evolution of the transmission with respect to the number of period. Going 191 from 20 periods to 80 periods, the resonance wavelength shift from 1549 nm to 1543 nm. This 192 is reasonable since it converges to the resonance position of the infinitely periodic structure 193 denoted by the green dashed line. Admitting that a minimum RD of 40% is necessary to ensure 194 a proper modulation, we note that starting from 50 periods, the resonance properties become 195 sufficiently relevant to ensure the good modulation thanks to its significant RD and Q factor. This 196 corresponds to a footprint of the structure as small as about $L=32.5 \,\mu\text{m}$. On the other hand, the 197 table 2 shows the characteristics of the resonances for each number of periods. Similarly to what 198 is presented in Fig.5, starting from 50 periods, the variation of the resonance properties becomes 199 very small, revealing the convergence to almost stable values. 200

Table 2. Details of the resonance properties with respect to the number of periods N.

Ν	$\lambda_{ m res}$	Q-Factor	RD
20	1548.80 nm	56.6	10.26%
30	1547.08 nm	126.3	19.6%
40	1546.04 nm	164.2	30.1%
50	1545 nm	217.47	39.28%
60	1544.76 nm	268.84	44.98%
70	1544.16 nm	273.73	47.59%
80	1543.65 nm	273.97	49.73%

In order to compare the performance of our modulator with other modulators available in the literature, we rely on the voltage-length product of the modulator expressed by the product V_{d} ·L, where V_{d} is the driving voltage of our structure and L the active length of the structure. If we consider a finite structure with 60 periods ($L = 39 \mu m$) and V_{d} 0.075 V or 0.2 V, we reach a voltage-length product of about 2.925×10^{-4} V·cm or 7.8×10^{-3} V·cm, respectively. In both cases, our voltage-length product is more than two order of magnitude smaller than other LN EO modulators [13, 15, 33]. In addition, a comparison table was provided in table 3 to benchmark all

Table 3. Comparison of modulator metrics: switching voltage, voltage-length product (V-L), ER and modulation tuning.

Туре	Switching Voltage (V)	V-L (V·cm)	ER (dB)	Modulation Tuning	Reference
MZI	1.4	2.8	30	N/A	[13]
MZI	2.3	2.3	30	N/A	[13]
MZI	4.4	2.2	30	N/A	[13]
Micro-Ring	9	1.8	10	7 pm/V	[31]
Metasurface	100	N/A	4.7	20 nm/V (GMR)	[34]
Our structure	0.075/ 0.2	2.925×10^{-4} / 7.8 × 10 ⁻³	4.7/ 6.7	14.35 nm/V	This work

207

208 relevant metrics.

209 4. Conclusion

Our theoretical studies reveal the opportunity to develop an EO modulator with a minimized driving voltage $V_d = 75$ mV and a reduced footprint of L = 39 µm based on the well-known EO effect in LiNbO₃, Pockels effect. We achieved a high sensitivity up to 14.35 nm/V and a minimized voltage-length product of about 2.925×10^{-4} V·cm with our 2D metasurface-based proposed structure. We reach a new horizon since, for the best of our knowledge, the deduced $V_d.L$ is the lowest in the literature and in the market.

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221 Disclosures

²²² The authors declare no conflicts of interest.

223 Data availability

Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

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