Conicity and depth effects on the optical transmission of lithium niobate photonic crystals patterned by focused ion beam

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Abstract: We report on novel focused ion beam fabrication techniques that can greatly improve the optical performance of photonic crystal structures. The finite depth and conicity effects of holes and trenches in Lithium Niobate (LN) photonic crystals have been theoretically analyzed, showing that the conicity causes refraction into the bulk sample, resulting in high transmission loss and no useful spectral features. The techniques for reducing the conicity angle from 25° to 5° were explained for the focused ion beam (FIB) milled structures.

References and links

11. Srico Inc., 2724 Sawbury Blvd., Columbus, OH 43235, USA.

1. Introduction

The typical length of conventional electro-optical modulators is 5-10 cm, requiring longer waveguides (WGs) and causing more transmission losses. Photonic crystals (PCs) as small as 10 µm can provide forbidden and permitted bands in optical wavelengths, leading to much smaller volume devices such as modulators or sensors [1]. Electro-optic properties of LiNbO$_3$ (LN) make it an ideal substrate for the fabrication of these PC devices. The small footprint of the PC structures shortens the required WG length and reduces the transmission losses.

It is challenging to fabricate reproducible and deep (sub-micron) structures [2–4] with conventional dry and wet etching methods in LN. Focused ion beam (FIB) is a direct nano-patterning route that has been used to fabricate different photonic device structures [5–7]. The milling beam size ranges from a few nanometers up to a few microns, which enables the fabrication of sub-micron sized structures. Typically Ga$^+$ ions are focused to a small spot size and accelerated up to a few tens of kilovolts. The material hit by Ga$^+$ ions is sputtered away. Fabrication of high-aspect ratio structures by FIB milling is challenging as the LN re-sputters, causing conical cross-sections and finite depths. These finite depths leading to conicity can drastically affect the performance of PC structures.

In this paper, we show theoretical and experimental results on how conicity can change the optical performance and the spectrum of PC structures. In order to reduce conicity, gas assisted etching for two dimensional PC (2D PC) structures were used and we observed slightly reduced conicity. One dimensional PC (1D PC) structures gave better results but our simulations have shown that the reduction of conicity was not enough to get the anticipated spectrum in bulk LN.

2. 2D photonic crystal design, fabrication and simulations

We designed 2D PC structure using triangular lattice of holes with a periodicity of 930 nm and radii of 325 nm. Finite Difference Time Domain simulations were performed in 2-dimensions with the MEEP software at Nanohub computational facilities [8–10]. Uniform cylindrical holes were assumed along the Z direction, thus the initial simulation was performed in two dimensions in the XY plane (Fig. 1(c)). As shown by the inverse triangle black curve in Fig. 1(a), the transmission spectrum had a dip around 1.6 microns. Based on these parameters, 2D PCs in LN WGs were fabricated (Fig. 1(b)).
FIB patterning was done on bulk LN substrates provided by SRICO Inc \cite{11}. These bulk samples have annealed proton exchange (APE) WGs which can support transverse electric (TE) modes. The widths of the WGs used for patterning varies from 5 to 7 microns to ensure single-mode transmission for the C-band laser source. The WGs had a pair of aluminum or gold coplanar electrodes for electro-optic measurements. These electrodes were also helpful in the alignment of the WG with the PC pattern. Using lower accelerating voltages enabled the scanning electron microscope (SEM) imaging of the WGs. Tilt correction helped the alignment of the WG in the horizontal direction without using alignment marks. Au-Pd was sputter coated on the substrates in order to avoid charging. This coating is needed to select the region of interest with SEM imaging. However, WGs are not visible after switching to ion-beam imaging due to this coating. Thus, a low dose ion bombardment of the region is required to remove the Au-Pd coating in order to make the WGs visible prior to PC patterning. Two different FIB systems were used for patterning: Helios Nanolab\textsuperscript{TM} DualBeam\textsuperscript{TM} and Zeiss NVision 40. These two systems utilize different pattern generation and gas injection systems. Both equipments use Ga\textsuperscript{+} ions and the focused beam diameter changes from a few nanometers up to a few microns depending on the beam current that varies from a few pA up to 40 nA. The patterns were etched using raster mode. Our test patterns were fabricated with variable dwell times, ranging from 0.2 \(\mu\)s to 1 \(\mu\)s, resulting in total time ranging from 5 s to 20 s. The test structures were also fabricated with variable beam currents but did not require beam drift correction. Figure 1(b) shows the SEM image of the triangular pattern written on the WG.

Optical transmission spectrum of this 2D PC structure is shown by the red solid curve in Fig. 1(a). The targeted dip at 1.6 microns in the simulation was not obtained experimentally. The cross section of the holes were analyzed by FIB milling and SEM imaging; the holes had truncated conical cross sections and depths less than 2 microns with conicity of 25° (Fig. 2(a)). Three dimensional simulations were performed to test the effect of conicity and finite depth. The simulated transmission spectrums of one- and two-micron deep conical holes are depicted in Fig. 1(a). The stop bands were not observed and the cones did not have useful spectral features.
In order to reduce conicity and to mill deeper, dwell time needs to increase which will result in larger radii holes. It is well known that LN is chemically inert to etching. It has been shown that Xenon Difluoride (XeF$_2$) assisted FIB milling of Si [12] and Quartz [13,14] enhances the milling quality in terms of conicity and depth. XeF$_2$ can increase the material removal rate by reducing the re-deposition effects and by more efficient chemical etching.

In our tests, XeF$_2$ improved the milling rate and enhanced the aspect ratio of the holes in LN. For this test, a fixed ion beam current of 150 pA, which gives a spot size of around 30 nm, was used. The effect of varying dwell times on the conicity and depth was tested. As seen in the SEM image of Fig. 2(a), for a dwell time of 20 seconds, the maximum milling depth was around 1.2 microns with a truncated conical cross-section. However with XeF$_2$, the milling depth increased to 2.1 microns with a conical well cross-section (Fig. 2(b)).

Gas assisted etching reduces the milling time; however, this option is not available in most FIB instruments. Thus, it is still possible to optimize the milling current and achieve critical hole-array dimensions without XeF$_2$ assisted etching in the shortest patterning time.

When shorter dwell times per hole but relatively higher beam currents (~460 nA) were used, the holes tend to have a different conicity that resembled an inverted tear drop shape (Fig. 3). Using shorter dwell times is important when large area patterns are desired in order to complete the milling in a reasonable time.

The finite-depth and the conicity have dramatic effects on the performance of PC devices in bulk LN. Lack of depth and increased conicity cause loss of pass and stop bands, and the attenuation due to refraction into the bulk substrate [15]. However, FIB milling leads to conicity because it is a kinetic mechanism. Therefore, the hole depths are limited due to re-sputtering effects because it is harder to remove the material from the bottom of a deeper hole. In order to get holes with good circularity and high depth, a line-defect PC pattern with various beam currents as in Fig. 4 was milled.
When switched from high to low beam current the aspect ratio of the holes increased allowing smaller holes with higher depths (Figs. 4(b) and 4(c)). We also used entity repeat function, which etches the entire array in layers, completing one full pass, and repeating across the same space until the pattern is complete. This results in structures of improved circularity and greater uniformity across the pattern. However, this method also increases the patterning time.

Gas assisted milling and patterning with low beam currents helped to get holes with low conicity and slightly larger depths but this still does not entirely solve the conicity problem. In order to obtain functional PC devices in bulk WGs, deeper holes with minimum conicity are needed. However 1D PCs have more potential in this respect due to extra degree of freedom for the material to be removed.

3. One dimensional photonic crystal design and conicity analysis

1D PC devices on WGs in bulk LN crystals were also designed, fabricated and tested. Hole and/or trench depth and conicity also have very significant effect on light propagation through 1D PC structures. One simple 1D PC design is a Bragg grating, which has been used in various applications such as optical filters and more recently in electric field sensing [16]. Here, the numerical analysis results of the conicity and depth effects on a Bragg grating structure using Finite Element Method (FEM) are presented. The trench pitch was set to 1 µm and compared to a structure without conicity and to one with a 5 degree conicity (Fig. 5(a)).
Light propagation of 1.2 μm in Bragg gratings of varying depth from 1 to 3 μm

Fig. 5. Bragg gratings with varying trench depths from 1 to 3 microns.

This angle was determined from the analysis of the SEM images of cross-sectional cuts of trenches. In the simulations the APE WG had an index of 2.148 and the index of the bulk LN was 2.138. Perfectly matched layers (PMLs) were used as the structure boundaries. One simple 1D PC design is a Bragg grating which have been used in various applications such as optical filters and more recently in electric field sensing [16]. In order to satisfy the Bragg condition the period $\Lambda$ must satisfy:

$$\Lambda = \frac{m\lambda}{2n}$$

Where $m$ is the grating order, $\lambda$ is the free space wavelength and $n$ is the refractive index [17]. In our designs, grating orders are 1 and 3 that give the periodicity of 360 and 1080 nm for LN ($n = 2.138$). The bandwidth is given by the following equation:

$$\Delta \lambda = \frac{\lambda_B^2}{nL} \sqrt{1 + \left(\frac{\kappa L}{\pi}\right)}$$

Where $\kappa$ is the coupling efficiency, $\lambda_B$ is the Bragg wavelength, $L$ is the overall grating length [18]. Using this equation, the grating length was calculated to be at the order of 100 to 200 μm.
for a bandwidth of 10 µm - the longer the device the smaller the bandwidth. The milling of these structures requires the beam to be swept along the direction of the linear cut, which brings an extra freedom for the material to be removed. The conicity angle of these linear cuts was lower compared to holes and their depth was as high as 5 µm depending on the trench width.

The panel b of Fig. 5 depicts the field images of the Bragg gratings with varying trench depths from 1 to 3 µm; for a trench depth of 1 µm, conicity had no influence on the transmission due to the finite trench depth. As shown in Fig. 5(c), the transmission spectrum did not display useful features and the transmission loss was not significant. This suggests that PCs with shallow depth structures are not ideal for the fabrication of functional devices on bulk LN. As the trench depth was increased to 2 µm, the transmission of the structure without the conicity displayed spectral dips up to several dBs. However, these features disappeared when the structure had a conicity of 5 degrees. As the trenches cut through the WG, the transmission became very small for a structure with 5 degree conicity. While the structure without conicity showed a clear broad band gap of more than 20 dB from 1.4 to 1.7 µm, the same structure with conicity of 5 degrees only showed significant transmission loss with no useful features.

This conicity analysis shows that, even with 1D PC, conicity has dramatic effect on transmission of light. These theoretical analysis results were used in designing and fabricating 1D PC structures including Bragg gratings [19–21] and Fabry-Perot [22] cavity structures (Fig. 6).

![Fig. 6. (a, b) Bragg gratings with periodicity of 1.876 microns (a) and 1.800 microns (b) Both are patterned with different beam current. As expected, lower beam gives finer trench width. (c) Fabry-Perot 1D PCs patterned on 3 different LN WGs. Each cavity has a gap of 40, 60 and 80 microns. (d) The inset SEM image shows one side of Fabry-Perot PC acting as a mirror. (e) Cartoon representation of light input and output through the PC structure along the WG.](image)

4. Electro-optical measurements

Electro-optic measurements were performed on the 1D PC structure (Fig. 6(a)). The periodicity of the air trenches was 1.876 micron. There were 20 air trenches in this structure giving 36 microns of device length. We measured the transmission spectrum by butt-coupling two polarization maintaining fibers at the input and output of the WG (Fig. 6(e)).
The structure was tested in the 1510-1580 nm range with a tunable laser source (SANTEC TSL-210H). An in-line fiber polarizer was used to externally polarize the laser output. We aligned the TE polarization parallel to the sample surface. Both ends of the input and the output fibers and the sample edges had angle-cuts to reduce reflections. An InGaAs photo detector in current mode measured the output signal. The curve with open squares in Fig. 7 shows the transmission spectrum of the periodic air trenches at zero DC bias. The spectrum shifted about 12 nm to the right when 10 V DC bias was applied to the electrodes. The intensities of the individual data points are, in general, increased by varying magnitudes along with the spectral shift.

![Graph showing transmission spectrum with applied voltage.](image)

**Fig. 7.** Electro-optical measurements of periodic air trenches (Bragg grating) in LN WG.

Although the structure does not fit well with our simulation/theoretical predictions, electro-optical measurements show that it responds well to electric field that is a result of the applied voltage to its electrodes. In our case the electrode separation is 10 microns and the electric field is less than $10^6$ V/m. The overall transmission loss in these 1D PC structures was recorded as 30 dB which inhibits their use in practical applications. This high loss is due to scattering of the field into bulk substrate as depicted in the simulated field images for trenches with conical cross sections. (Fig. 5(c), right panels).

1D PC structures have enabled the fabrication of deeper trenches but the simulated spectrum was not obtained in the optical measurements due to conicity of the trenches (around 5°). In order to improve the conicity of these air trenches, a new approach was developed using side pockets.

### 5. Fabrication of deeper air trenches with less conicity

Finding the optimum dose and ion beam probe width is always a compromise between time and exposure area in FIB milling. A smaller beam was used with a small probe size for finer structures which resulted in longer patterning time. In order to further decrease the conicity and to fabricate deeper air trenches, “side-pockets” were milled on both sides of the WGs prior to air trench milling. These pockets facilitated the removal of the material in the direction of beam sweep. As shown in Fig. 8, the side pockets not only reduce the air trench conicity but also increase their depths.
Fig. 8. The cross-sectional view of air trenches. (a) The cross-sectional view when the side pockets are milled prior to the milling of trenches by using beam exposures similar to trenches in (b). The cuts are of reduced conicity and greater depth.

This method was used to fabricate 1D PC structures and FP resonators with multiple cavities as depicted in Fig. 9. These are Bragg gratings and Fabry-Perot structures with side pockets. All the structures are centered in the WGs.

Fig. 9. (a) 1D PC and (b) two cavity Fabry-Perot structure with side-pockets. (c) A close-up view of Fabry Perot mirrors.

Side pockets reduced conicity but optical performance degraded. This could be attributed to the loss of the transmitted light into the side pockets or because of the large width of the trenches. But it is worth mentioning that side pockets have increased the uniformity and the depth of the trenches.

6. Summary
Bragg gratings and Fabry-Perot type structures in WGs were patterned using FIB. Our simulations showed that conicity has a significant impact on the optical transmission. Cross-sectional SEM images of trenches were analyzed and compared with the experimental results. Although the optical measurements do not match well with the simulation results, mostly owing to the conicity, electro-optical effect is well demonstrated. In order to reduce the conicity even further a new pocketing technique was developed, which allows the milling of deeper structures with less conicity and with higher uniformity. But the optical losses have also increased, which could be due to the light lost into the pockets and the width of the trenches.

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