Simulation of Ti-indiffused lithium niobate waveguides and analysis of their mode structure

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Abstract. Simulation of Ti-indiffused waveguides on LiNbO₃ is described. The influence of diffusion conditions and technological parameters on the waveguide mode structure is considered. Boundaries of multimode, single-mode, and single-mode polarizing regimes of operation are defined.

1. Introduction

In integrated optics, where optical and optoelectronic devices are fabricated on a single wafer, optical waves propagate in the waveguides formed in the surfactant area of the wafer material. Since waveguides are basic elements of every integrated optical device, their properties are of a great importance. In order to fabricate an integrated optical device, it is necessary to know, for example, the waveguide size, its optical losses per unit length, and its eigen mode structure. These properties depend on the method of fabrication and, hence, on the technological parameters used in the fabrication. The waveguide properties can be tailored to specific applications by varying technological parameters. In addition, since production of devices demands reproducible results, it is important not only find the fabrication parameters under which the desired waveguide properties can be obtained, but also estimate the allowable deviations from these parameters which will not lead to a deterioration of necessary waveguide properties.

The influence of technological parameters on the waveguide properties can be studied experimentally or theoretically (analytically or numerically). However, the first approach encounters difficulties because of a long production cycle of experimental waveguides. It is much more suitable to define the necessary range of technological parameters and only then to test experimentally whether the calculations have given a correct result.

Nowadays lithium niobate (LiNbO₃) is a widely spread material for integrated optics [1, 2]. This crystal is very suitable as a wafer because of the presence of electrooptical properties (which is important for fabrication of modulators) [3], its transparency in the visible and near infrared spectral ranges, piezoelectric effect [4], and applicability in nonlinear optics [5]. There are two basic technologies for fabrication of optical waveguides on lithium niobate with low losses (<0.1 dB/cm) [1]. The first method, i.e., titan indiffusion, leads to an increase in both the ordinary and extraordinary refractive indexes in this birefringent crystal. The second method, i.e., the so-called proton exchange, increases the extraordinary refractive index alone, and thus allows one to create polarizing waveguides [2, 6].

Both methods produce channel waveguides with a gradient refractive index distribution and, therefore, the waveguide parameters cannot be analyzed analytically. To get a proper understanding of
the influence of technological parameters on the characteristics of the waveguide being fabricated, numerical simulation is needed. This report is devoted to the simulation of Ti-indiffused waveguides.

2. Ti:LiNbO$_3$ waveguides

Indiffusion of Ti is a traditional method of fabrication of LiNbO$_3$ waveguides [2]. In this technique, a metal strip is sputtered on a crystal surface and then is annealed at temperatures near 1000°C (figure 1).

![Figure 1. Fabrication of Ti:LiNbO$_3$ waveguides](image)

The result of the diffusion process for the x-cut crystal orientation can be described analytically in terms of error functions as

$$C(x, z) = C_0 \left[ \text{erf} \left( \frac{h + x}{\sqrt{4D_X t}} \right) + \text{erf} \left( \frac{h - x}{\sqrt{4D_X t}} \right) \right] \times \left[ \text{erf} \left( \frac{W/2 + z}{\sqrt{4D_Z t}} \right) + \text{erf} \left( \frac{W/2 - z}{\sqrt{4D_Z t}} \right) \right],$$

(1)

where $C$ is the Ti concentration, $D_Z$ and $D_X$ are the diffusion coefficients along the Z and X axes, respectively, $t$ is the annealing time, and $h$ and $W$ are the thickness and width of the sputtered Ti strip, respectively (figure 2).

![Figure 2. Crystal orientation (x-cut) and parameters of the sputtered Ti strip](image)

The change in the refractive index caused by the diffusion process [2] can be described by semi-empirical equations [7]

$$\Delta n_{o,e} (x, z, \lambda) = A_{o,e} (\lambda) [C(x, z)]^{\alpha_{o,e}},$$

(2)

where $A_{o,e}$ and $\alpha_{o,e}$ are unknown constants at a fixed wavelength.

Since the Ti indiffusion increases both the ordinary and extraordinary refractive indexes, it allows propagation of the orthogonally polarized TM and TE modes through the waveguide.
3. Simulation

To perform the simulation, the numerical finite element method in the COMSOL Multiphysics package was used.

The refractive index distribution which was necessary for the mode structure analysis could not be defined without knowing the numerical values of the constants used in expressions (1) and (2) \(D_x, D_z, \alpha_e, \alpha_o, A_e, A_o, C_0\). In order to find them, the experimentally captured mode field distributions were used (figure 3). They were obtained for a single-mode waveguide fabricated under technological parameters \(W=6 \, \mu m, h=100 \, nm, t=17 \, h\), and temperature \(T=1000^\circ C\), which yielded the waveguide sizes which were most suitable for optimum coupling to standard single-mode optical fibers. The constants were found through an iterative algorithm, so that the computed intensity distributions of the mode field (figure 4) matched the experimentally obtained ones (figure 3). The search and fitting were performed for the constants similar by the order of magnitude to those reported in the literature for other crystal orientations and annealing times [7].

![Figure 3. Experimentally captured intensity distributions for TE and TM modes](image)

Then the technological parameters were varied at a fixed wavelength (\(\lambda=1550 \, nm\)) and at the constants derived above \((D_x=D_z=0.19 \, \mu m^2/h, \alpha_e=0.69, \alpha_o=0.46, A_e(C0)=0.0121, A_o(C0)=0.0419)\), and the resulting mode composition was analyzed. To simplify the analysis we varied only two parameters, i.e., the Ti strip width and annealing time. The Ti strip height was fixed at a value of
100 nm, at which the experimentally fabricated waveguides had the lowest losses. The strip width and time of annealing were varied in the vicinity of 6 μm and 17 h, respectively. Results of simulation are presented in figure 5.

![Figure 5](image)

**Figure 5.** Results of simulation: dependence of supported modes on technological parameters (Ti strip width and annealing time). The blue circles correspond to the single-mode regime, the red squares mark the polarizing regime, and the asterisks are for the multimode regime.

4. Results

The analysis revealed how technological parameters affected the mode structure of waveguides. It was found that large widths of a sputtered metal strip and long annealing times resulted in multimode waveguides. If both parameters were decreased, the waveguides supported only one TE and one TM mode (a single-mode regime). A further decrease in the annealing time and strip width caused the TM mode cutoff, and the waveguides became polarizing. Such an influence of the technological parameters on the mode composition was caused by different ordinary and extraordinary refractive index distributions (figure 6) which were formed during the Ti indiffusion.

![Figure 6](image)

**Figure 6.** Computed distributions of refractive index increase for $n_e$ and $n_o$ at $z=0$ for a polarizing waveguide ($W=3$ μm, $t=9$ h) and for a single-mode waveguide with both the TE and TM modes ($W=5$ μm, $t=21$ h).
Therefore, it is possible to fabricate polarizing waveguides by using indiffusion of titan. This result is highly important because a single-mode polarizing regime of operation is necessary for production of such devices as amplitude modulators with a high extinction ratio and others. As mentioned in the Introduction, the polarizing properties are generally associated with proton exchanged waveguides.

To suppress the TM mode in single-mode Ti:LiNbO$_3$ waveguides, plasmon-polariton polarizers are employed at present, but such polarizers cause optical losses and a special technological step is needed to obtain polarizing properties [8]. The use of new Ti-indiffused waveguides that are originally polarizing is much more promising.

5. Conclusions
The simulation of Ti-indiffused waveguides on LiNbO$_3$ was described. The analysis of the effect of technological parameters on waveguide eigen modes was carried out. As an example, the influence of the Ti strip width and annealing time on the mode structure was investigated. The boundaries of multimode, single-mode, and single-mode polarizing regimes of operation were defined. The technological parameters for production of polarizing waveguides by Ti-indiffusion were estimated. The results obtained were found to be in good agreement with the experimental results. Our findings can prove useful for the development of integrated optical devices.

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