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IEEE Photonics Journal

An IEEE Photonics Society Publication

Volume 4, Number 5, October 2012

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DOI: 10.1109/JPHOT.2012.2217736 1943-0655/\$31.00 ©2012 IEEE





Refractive Index Profile in Photorefractive-Damage-Resistant Near-Stoichiometric Ti:Mg:Er:LiNbO₃ Strip Waveguide

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> DOI: 10.1109/JPHOT.2012.2217736 1943-0655/\$31.00 © 2012 IEEE

Manuscript received July 26, 2012; accepted September 4, 2012. Date of publication September 7, 2012; date of current version September 21, 2012. This work was supported in part by the National Natural Science Foundation of China under Projects 50872089, 61077039, and 61107056, by the Key Program for Research on Fundamental to Application and Leading Technology, Tianjin Science and Technology Commission of China under Project 11JCZDJC15500, and by the Specialized Research Fund for the Doctoral Program of Higher Education of China under Project 20100032110052. Corresponding author: D.-L. Zhang (e-mail: dlzhang@tju.edu.cn).

Abstract: Refractive index profile in photorefractive-damage-resistant near-stoichiometric (NS) single-mode Ti:Mg:Er:LiNbO₃ strip waveguide is constructed from the measured mode field distribution. Like the conventional congruent Ti:LiNbO₃ waveguide, the Ti-induced refractive index increase in the NS waveguide studied here follows a sum of two error functions in the width direction and a Gaussian function in the depth direction. Based upon the established index profile model, the mode sizes were calculated using the variational method and compared with the experimental results. The Ti-induced index increment at the NS waveguide surface was also evaluated according to the empirical relation previously reported for the conventional congruent Ti:LiNbO₃ waveguide and compared with the data deduced from the mode field distribution. All comparisons show good agreement, showing that the index model proposed is close to the practical scenario.

Index Terms: Near-stoichiometric (NS) Ti:Mg:Er:LiNbO₃ waveguide, refractive index profile, mode field distribution, variational method.

1. Introduction

Over the past years, a family of Ti-diffused Er:LiNbO₃ (Ti:Er:LN) waveguide lasers (amplifiers) and integrated devices operated in infrared regime have been demonstrated [1]–[10]. Because these devices were fabricated on a congruent LiNbO₃ substrate, the photorefractive effect not only limits both the pumping and operating wavelengths but also affects the performance of these devices more or less. The photorefractive effect is a result of the combination of two phenomena, i.e., the absorption of light by crystal defects leading to the formation of a space-charge field by the generated photocarriers and the subsequent modulation of the refractive index of the medium by this space-charge field via electrooptic effect. It is particularly serious in the visible regime and hence hinders development of new devices. To suppress this effect, two methods have been attempted previously.

One is by propagating along the optical axis of the crystal [3]. A disadvantage of this scheme is that it sacrifices the larger electrooptic coefficient r_{33} . Another method is by using ZnO-diffused waveguide on an Er:LN codoped with > 5 mol% MgO [5], [6]. However, a large amount of MgO doping causes difficulty in growing Er/Mg-codoped single crystals with the desired optical quality for device fabrication, while a congruent crystal doped with < 5 mol% MgO cannot effectively suppress the photorefractive effect. Moreover, for a Ti:Er:LN device, selective Er doping is a prerequisite for monolithic integration of active (optically pumped Er-doped) and passive (unpumped) devices on a same substrate to avoid reabsorption in unpumped Er-doped waveguides [1]-[7], [8]-[10]. Local Er doping in an LN crystal is usually realized via diffusion of Er metal or its oxide at the temperature close to the Curie point of the crystal (~1142 °C at the congruent point) [11], [12]. Heavy MgO doping results in extremely low Er diffusivity and solubility [6], [13], [14]. The previous studies have shown that a nearstoichiometric (NS) LN doped with lesser amount of MgO (> 0.3 mol%) can also effectively suppress the photorefractive effect [15]-[17]. Moreover, the NS LN also exhibits some other advantages over the congruent material such as remarkably lowered coercive field strength needed for the reversal of ferroelectric domain, larger electrooptic and nonlinear effects, etc. In addition, as we know, there are two kinds of often employed LN waveguides. One is the proton-exchanged (PE) waveguide, another is the Ti-diffused. The PE LN waveguide suffers from a series of problems such as the degradation of electrooptic coefficient and nonlinear optical susceptibility, copresence of complicated, protonconcentration-related multiple crystalline phase sublayers in the PE layer, negative effect on Er³⁺ electronic transition lifetime [18], low stability due to the high proton mobility, and larger waveguide loss. Instead, the Ti:LN waveguide is of a number of advantages over the PE waveguide such as lower loss, higher stability, retained crystalline phase, and, hence, the electrooptic, nonlinear, and Er³⁺ spectroscopic properties. All of the aforementioned problems concerning with PE waveguide can be avoided if the Ti:LN waveguide is employed. Thus, an NS Ti:Mg:Er:LN waveguide is promising for developing the photorefractive-damage-resistant devices. Its realization would open up with some new applications such as 980-nm-LD-pumped green upconversion and midinfrared (2.7 μ m) waveguide lasers, and various guasi-phase-matching devices based on periodically poled LN waveguide that may be pumped and/or operated in both visible and infrared regimes.

How to fabricate an NS Ti:Mg:Er:LN waveguide is a challenge. Over the past years, the authors have expended much effort to explore a way to the NS Ti:Mg:Er:LN waveguide. Several methods have been tried, and each suffers from one problem and another. The authors first tried the fabrication starting with a bulky Er/Mg-codoped congruent crystal and adopting the method of either Ti diffusion followed by post Li-rich vapor transport equilibration (VTE) or cowork of Ti diffusion and Li-rich VTE. However, neither is successful because the Li-rich VTE induces both micron-sized ErNbO₄ precipitation on crystal surface and MgO out-diffusion to crystal surface [19], which, together with the Li-rich VTE effect on crystal composition, results in the decline of refractive index near the crystal surface and, hence, no waveguiding in the Ti-diffused layer. The authors also attempted direct Ti-diffused waveguide fabrication on a bulky Er (1.0 mol%)/Mg (1.0 mol%)-codoped NS crystal. The ErNbO₄ precipitation took place also on the crystal surface. It is also not feasible that the fabrication starts with a singly MgO-doped congruent or NS crystal because the former case suffers from VTE inducing MgO out-diffusion and local Er-doping in an MgO-doped NS crystal is almost impossible. Recently, the authors have reported a feasible way to a photorefractive-damageresistant NS Ti:Mg:Er:LN strip waveguide [20]. The fabrication starts from a pure congruent LN crystal with a technological process in sequence of local Er doping, Mg/Ti pre-diffusion and post Lirich VTE. In our earlier paper [20], the waveguiding characteristics, mode field profiles, composition, crystalline phase and photorefractive effect of such NS waveguides have been studied. The results show that such waveguide is NS and single mode at the 1.5-µm wavelength, supports only transverse magnetic (TM) mode, has a loss of 1.4 dB/cm, and retains still the LN phase. The photorefractive effect in the NS waveguides was examined by monitoring the stability of the signal enhancement of small-signal $(1-\mu W)$ 1.531- μm input light under 980-nm wavelength laser diode pump power. The signal enhancement in the congruent waveguides drops significantly when the pump power exceeds 20 mW, showing that the optical damage is serious in the congruent waveguides. In contrast, for the NS Ti:Mg:Er:LN waveguides, the maximum signal enhancement is 2.8 dB/cm and is stable up to the maximum available coupled pump power of 216 mW, implying that these NS waveguides can withstand an light intensity of at least 10^{10} W/m² without the photorefractive damage appeared.

It is crucial to have the knowledge of the refractive index profile in the guiding layer of the NS Ti:Mg:Er:LN strip waveguide. As we know, the mode indices of a slab or planar waveguide can be measured using the standard prism-coupler method [21]. With the knowledge of measured mode indices, the refractive index profile in the planar waveguide can be constructed using the inverse Wentzel-Krames-Brillouin (IWKB) method [22], [23]. With the improved IWKB method [24]-[26], more accurate index profile could be obtained. For an index-graded single-mode strip waveguide, however, it is not easy to directly measure the index profile. The commonly adopted effective method is using secondary ion mass spectrometry (SIMS) technique to find the dopant concentration profile. The refractive index change profile can be calculated from the known relation between index change and dopant concentration. Although this method is precise and effective, the relation between index change and dopant concentration must be known in advance. For the conventional congruent Ti:LN waveguide, the relation between index change and Ti⁴⁺ dopant concentration is known [27], [28]. For the NS Ti:Mg:Er:LN waveguide studied here, however, the relation is unknown. It is unclear if the NS composition and the incorporation of multiple ions Er³⁺, Ti⁴⁺, Mg²⁺, and Li⁺ lead to a different relationship between the index change and the Ti⁴⁺ concentration. In the previous papers [29], [30], researchers have demonstrated another method used to construct the index profile in the conventional congruent single-mode Ti:LN strip waveguide. The method, based upon the measured mode field profile, is much simpler than the SIMS technique because the nearfield mode profile of the waveguide is obtained much easier than the relationship between the index change and the Ti⁴⁺ dopant concentration. Here, we employ this method to construct the index profile of the NS Ti:Mg:Er:LN strip waveguides studied here. Based upon the constructed index profile model, the mode size was calculated using the variational method and compared with the experimental data to examine the validity of the constructed index model. For the same purpose, the Ti-induced surface index increment was also evaluated using the empirical relation previously reported for the conventional congruent Ti:LN waveguide, and the evaluated result is compared with the data deduced from the mode field distribution.

2. Numerical Methods

2.1. Construction of Refractive Index Profile From Measured Mode Field Profile

The construction of refractive index profile from the measured mode field profile is carried out in a following way. For convenience, here, we consider an x-y Cartesian reference frame that is fixed at the center of the strip waveguide surface with the *x*-axis along the width direction and the *y*-axis pointing to the depth direction of the waveguide. At first, we define a normalized electric-field intensity profile on the waveguide cross section E(x, y) given by

$$E(x,y) = \sqrt{\frac{I(x,y)}{I_{\max}}}$$
(1)

where I(x, y) represents the measured 2-D light intensity profile of guided mode and I_{max} denotes the maximum light intensity.

It is assumed that the permeability of the medium is equal to that of the vacuum and the refractive index change is small; the Maxwell's equations are then approximated into the following 2-D scalar wave equation:

$$\left(\frac{\partial^2}{\partial x^2} + \alpha^2 \frac{\partial^2}{\partial y^2}\right) E(x, y) + \left[k^2 n^2(x, y) - \beta^2\right] E(x, y) = 0$$
(2)

where α is the factor that considers the anisotropy of the LiNbO₃ crystal [28]. For a Z-cut LiNbO₃ substrate, like the one studied in this paper, $\alpha = 1$ for the transverse electric (TE) mode and n_e/n_o

for the TM mode (n_e and n_o are the extraordinary and ordinary refractive indices of the substrate material, respectively.). In (2), n(x, y) is the 2-D refractive index profile on the waveguide cross section, $k = 2\pi/\lambda$ is the propagation constant in free space, and $\beta (= kN_{eff})$ is the effective propagation constant in the waveguide, where N_{eff} is the effective refractive index of the guided mode.

The approximate expression of n(x, y) is then given by

$$n(x,y) = \sqrt{N_{\text{eff}}^2 - \frac{1}{k^2 E(x,y)} \left(\frac{\partial^2}{\partial x^2} + \alpha^2 \frac{\partial^2}{\partial y^2}\right) E(x,y)}.$$
(3)

With the known mode index and the measured light intensity profile of the guided mode, one can numerically solve for the index profile of the material from (3).

2.2. Mode Size Calculation by Variational Method

To examine the validity of the refractive index model proposed, we have calculated the mode sizes using the variational method and compared the calculated results with the experimental data. For an arbitrary order mode guided in a conventional congruent Ti:LiNbO₃ strip waveguide, the normalized field distribution $E_{nm}(x, y)$ can be expressed as

$$E_{nm}(x,y) = \frac{2}{\sqrt{W_x W_y}} \psi_n\left(\frac{\sqrt{2}x}{W_x}\right) \psi_{2m+1}\left(\frac{\sqrt{2}y}{W_y}\right)$$
(4)

$$\psi_j(\xi) = \frac{1}{\sqrt{2^j j! \sqrt{\pi}}} \exp\left(-\frac{\xi^2}{2}\right) H_j(\xi)$$
(5)

where W_x and W_y are the so-called mode sizes, $H_j(\xi)$ is the *j*th-order Hermite polynomial, and n and 2m + 1 are the mode orders in the *x* and *y* directions, respectively. For the single-mode strip waveguide studied here, only the fundamental mode is considered, i. e., m = n = 0.

Left-multiplying two sides of (2) by E(x, y) and integrating over the xy plane, one can obtain the following integrating equation used for variational analysis:

$$\beta^{2} = \frac{\iint E(x, y) \left(\frac{\partial^{2}}{\partial x^{2}} + \alpha^{2} \frac{\partial^{2}}{\partial y^{2}}\right) E(x, y) dx dy + k_{0}^{2} \iint n^{2}(x, y) E^{2}(x, y) dx dy}{\iint E^{2}(x, y) dx dy}.$$
(6)

Inserting the known index profile and field distribution into (6), one can obtain an expression of β^2 with regard to W_x and W_y . By using the variational method, one can obtain the optimum values of W_x and W_y corresponding to the largest value of β^2 , namely, β_m^2 . Then, the corresponding effective refractive index is given by

$$N_{\rm eff} = \frac{\lambda}{2\pi} \beta_m. \tag{7}$$

3. Results and Discussion

3.1. Model of Refractive Index Profile in Waveguide Layer

As described in the introduction part, the studied NS Ti:Mg:Er:LN strip waveguides with an initial Ti-strip width of 4–7 μ m are single mode at the 1.5- μ m wavelength and only well support the TM mode [20]. The near-field pattern of the TM single-mode guided in the studied NS strip waveguides has been measured at the 1.5- μ m wavelength. Fig. 1(a) shows the captured near-field patterns of the TM-mode guided in the 4-, 5-, 6- and 7- μ m-wide NS Ti:Mg:Er:LN strip waveguides at the 1.5- μ m wavelength. Fig. 1(b)–(e) representatively shows the light intensity profiles (full squares) along the width and depth directions of the 4- [(b) and (c)] and 7- μ m-wide [(d) and (e)] waveguides. Analysis shows that, like the conventional congruent Ti:LN strip waveguide, the light intensity of the mode guided in the NS guide under study follows well a Gauss function A_xexp[$-2(x/W_x)^2$] in the width



Fig. 1. (a) Near-field patterns of TM mode guided in the 4-, 5-, 6- and 7- μ m-wide NS Ti:Mg:Er:LN strip waveguides at 1.5 μ m. (b)–(e) Light intensity profiles (full squares) along the width and depth direction of the 4- μ m-wide [(b) and (c)] and 7- μ m-wide [(d) and (e)] waveguides. The solid lines in (b)–(e) represent the fitting results using a Gaussian or Hermite-Gaussian trial function. (f) Measured (full squares or circles) and calculated (solid lines) mode size W_x and W_y versus Ti-strip width W.



Fig. 2. Refractive index change profile along (a) the width and (b) the depth direction of the 7- μ m-wide NS Ti:Mg:Er:LN strip waveguide calculated from the measured width or depth mode field profile.

direction and a Hermite–Gauss function $A_y y^2 \exp[-2(y/W_y)^2]$ in the depth direction. This corresponds to the case of m = n = 0 in (4). The solid lines in Fig. 1(b)–(e) represent the fitting results using a Gaussian or Hermite–Gaussian trial function. Fig. 1(f) shows the mode size W_x (full squares) and W_y (full circles) measured as a function of the Ti-strip width W. Similar to the case of conventional congruent Ti:LiNbO₃ waveguide, the mode size increases with the decrease of W as a result of approaching the cutoff region.

Both the width and depth mode-field profiles were used to deduce the refractive index change profile using the (3). Note that, for a TM mode guided in a waveguide defined on a Z-cut LiNbO₃ substrate, the extraordinary refractive index is concerned. Since the mode field profile is well fitted by a Gaussian function in the width direction and a Hermite–Gauss function in the depth direction, it is more convenient to use the fitting expressions $A_x \exp[-2(x/W_x)^2]$ and $A_y y^2 \exp[-2(y/W_y)^2]$ to deduce the profile of refractive index change Δn_e . As a representative, in Fig. 2(a) we show the deduced refractive index change profile along the width direction of the 7- μ m-wide NS Ti:Mg:Er:LN strip waveguide. Fig. 2(b) shows the case along the depth direction of the waveguide. It is found that, like the conventional congruent Ti:LN waveguide [28]–[30], the index change on the surface of the NS guide studied here also follows a sum of two error functions, given by:

$$\Delta n_e(x,0) = \Delta n_e(0,0) \times g(2x/W)$$

= $\Delta n_e \times \{ \operatorname{erf}[(W+2x)/(2d_x)] + \operatorname{erf}[(W-2x)/2dx] \} / 2\operatorname{erf}[W/(2d_x)]$ (8)

where *W* is the initial Ti-strip width having a value of 7 μ m; $\Delta n_e(0,0)$, abbreviated as Δn_e , is the maximum index increment at the waveguide surface, it has a value similar to 0.0206 at the 1.5 μ m wavelength; and d_x is the fitting width parameter that has a value of 5.4 μ m. Like the conventional

congruent Ti:LN waveguide, the index change profile in the depth direction follows a Gaussian function given by

$$\Delta n_e(0, y) = \Delta n_e(0, 0) \times f(y/d_y) = \Delta n_e \times \exp\left[-(y/d_y)^2\right]$$
(9)

where d_y is the fitting depth parameter that has a value of 5.3 μ m, and the surface index increment at the 1.5 μ m wavelength $\Delta n_e(0,0)$ has a value of 0.0211, which is reasonably in good agreement with the value obtained from the width profile, 0.0206.

Then, the 2-D extraordinary refractive index profile $n_e(x, y)$ in the NS Ti:Mg:Er:LN strip waveguide studied can be written as

$$n_{e}(x,y) = \begin{cases} 1, & y < 0\\ n_{e}^{sLN} + \Delta n_{e}(0,0)g(\frac{2x}{W})f(\frac{y}{d_{e}}), & y \ge 0 \end{cases}$$
(10)

$$g\left(\frac{2x}{W}\right) = \frac{1}{2\mathrm{erf}\left(\frac{W}{2d_x}\right)} \left[\mathrm{erf}\left(\frac{W+2x}{2d_x}\right) + \mathrm{erf}\left(\frac{W-2x}{2d_x}\right)\right]$$
(11)

$$f\left(\frac{y}{d_y}\right) = \exp\left[-\left(\frac{y}{d_y}\right)^2\right] \tag{12}$$

where the Ti-induced surface index increment at x = y = 0, $\Delta n_e(0,0)$, should take the mean value of 0.0211 and 0.0206, i. e. 0.0209 at the 1.5- μ m wavelength. The waveguides with other initial Ti-strip widths of 4, 5, and 6 μ m were analyzed in a similar way. Similar profile characteristics and similar fitting parameter values of $\Delta n_e(0,0) = 0.020 - 0.025$, $d_x = 5.3 - 5.6 \mu$ m, and $d_y = 5.1 - 5.4 \mu$ m were obtained. These parameter values are independent of *W*, consistent with the case of conventional congruent Ti:LN waveguide. Taking all sources of error into account, the uncertainty of the index model is conservatively estimated to be within ±25%.

In (10), n_e^{sLN} is the extraordinary index of the substrate. It has been demonstrated that the Li₂O content over the surface depth range of 20 μ m, which is thicker than the waveguide layer, is NS and approximately homogeneous having a value about 49.8 ± 0.1 mol% [20]. Moreover, the MgO within the surface depth range of 20 μ m is also homogeneous and has a concentration of ~2 mol% [20]. This means that the 2 mol% MgO-doped NS LiNbO₃ should be considered as the substrate of the waveguide. On the basis of the Sellmeier coefficients reported for the 2 mol% MgO-doped NS LiNbO₃ crystal [31], the extraordinary substrate index n_e^{sLN} is evaluated as 2.1235 at the 1.5 μ m wavelength (2.2098 for the case of ordinary ray).

3.2. Verification of Refractive Index Profile Model by Variational Method

It is essential to examine the validity of the refractive index profile model proposed. This can be done by calculating at first the mode sizes on the basis of the supposed refractive index profile and the variational method, and then comparing the calculated results with the experimental data.

With the small term ignored, (10) can be approximately written as

$$n_{e}^{2}(x,y) \approx \begin{cases} 1, & y < 0\\ \left(n_{e}^{sLN}\right)^{2} + 2n_{e}^{sLN} \Delta n_{e}(0,0) g\left(\frac{2x}{W}\right) f\left(\frac{y}{d_{y}}\right), & y \ge 0. \end{cases}$$
(13)

Inserting (4) in case of m = n = 0 and (13) into (6), one can obtain

$$\beta_{00}^{2}(W_{x}, W_{y}) = k_{0}^{2} \left(n_{e}^{sLN} \right)^{2} + \frac{64k_{0}^{2}}{\sqrt{\pi}} n_{e}^{sLN} \Delta n_{e}(0,0) Q_{0} R_{0} - \frac{1}{W_{x}^{2}} - \alpha^{2} \frac{3}{W_{y}^{2}}$$
(14)

$$Q_0 = \frac{1}{W_x} \int_0^{+Z_x} g\left(\frac{2x}{W}\right) \psi_0^2 \left(-\frac{\sqrt{2}x}{W_x}\right) dx$$
(15)

$$R_0 = \frac{1}{W_y^3} \int_0^{+\infty} f\left(\frac{y}{d_y}\right) \exp\left(-\frac{2y^2}{W_y^2}\right) y^2 dy.$$
(16)

Note that the upper limit of the integral in (15), i.e., z_x , denotes the *x* coordinate where g(2x/W) = 0. Equation (14) is a binary function with regard to the two elements W_x and W_y . By applying the variational method to (14), one can solve for W_x and W_y . The solution is actually the problem of extremum of a binary function. The calculated W_x and W_y of the TM mode guided in the 4-, 5-, 6- and 7- μ m-wide NS Ti:Mg:Er:LN waveguides are comparatively illustrated in Fig. 1(f) (see the solid lines). One can see that the theoretical results of the mode sizes are in good agreement with the experimental data. The difference of each other is only within $\pm 10\%$, indicating that the refractive index profile model constructed from the measured mode field distribution is close to the practical scenario.

In addition, an empirical relation between the Ti-induced surface index increment and the diffusion parameters has been previously reported for the conventional congruent Ti:LN waveguide [27]. By using this empirical relation, one may roughly evaluate the Ti-induced surface index increment of the NS waveguide studied here and then compare with the result deduced from the mode field distribution. The empirical relation is conducted with the wavelength considered and the diffusion parameters of initial Ti-strip thickness and diffusion depth, which are 1.5 μ m, 169 nm, and 5.3 μ m, respectively, for the NS waveguide studied here. Inserting these parameter values into the empirical relation, one can find that the surface extraordinary index increment $\Delta n_e(0,0)$ is ~0.024, which can be approximately considered as the same as the value deduced from the mode field distribution, 0.020–0.025, as the ±25% error of the index model is taken into account. This agreement provides further evidence for the conclusion that the refractive index profile model proposed is valid for the NS waveguide studied here.

4. Conclusion

The refractive index profile model has been constructed for the photorefractive-damage-resistant single-mode NS Ti:Mg:Er:LN strip waveguide from the measured mode field distribution. Like conventional congruent Ti:LN waveguide, the index increment in the NS waveguide follows a sum of two error functions in the width direction and a Gaussian function in the depth direction. The model is considered as accurate within $\pm 25\%$. The mode sizes calculated on the basis of the proposed index model are in good agreement with the measured values within the error. Moreover, the Ti-induced surface index increment value evaluated according to the previously reported empirical relation can be approximately considered as the same as the data deduced from the mode field distribution taking into account the $\pm 25\%$ error of index model. These agreements confirm the validity of the index profile model proposed.

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