Study of Refractive Index and Birefringence Variation near the Surface of LiNbO₃ Open Type Optical Waveguide using Point Dipole Approximation

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Abstract. In view of the immense use of LiNbO₃ (LN) in the Photonic industry, a need arises to develop a theory to study the variation of Refractive Indices near the surface of LN device. The “Local” fields as experienced by ions on or near the surface of a dielectric medium ought to be different from those in the interior, thus one expects a Refractive Index variation near the surface of the material. In the studies involving thin films and optical waveguides, this variation could possibly alter the propagation characteristics. The variation of ordinary and extraordinary refractive indices \(n_o\) and \(n_e\) from the surface to the interior of depth 69.315Å near the surface for \(X\)-cut and \(Z\)-cut LN waveguides are evaluated using theoretical Point Dipole Approximation (PDA) method. For an \(X\)-cut waveguide, \(n_o\) is found to decrease from 2.9696 on the surface to 2.2864 in the interior whereas, \(n_e\) is found to increase from 1.4849 to 2.2024. The birefringence \((dn=ne-n_o)\) is negative and observed to be increase from -1.4847 to -0.0840. For a \(Z\)-cut waveguide, \(n_o\) is found to increase from 1.8046 to 2.2864 whereas \(n_e\) is found to decrease from 2.7005 to 2.2024. Here the birefringence is positive, decreasing from 0.8958 to zero to a depth of 60.5Å and further decreasing to -0.0840 to a depth of 69.315Å. It is observed that the variation of refractive indices \(n_o\), \(n_e\) and \(dn\) variation with depth near the surface for both the cases are quite opposite in nature. This is primarily due to the dipole orientation and their relative distributions in the lattice being different for the two directions of the electric vectors of light as is evident from the values.

Keywords: Refractive Index, Birefringence, LiNbO₃ Open Type Waveguide, Point Diople Approximation.

1. Introduction

Lithium Niobate (LiNbO₃ / LN) is a well known ferroelectric material for its excellent nonlinear-optic, electro-optic, acousto-optic, piezoelectric, and pyroelectric properties which makes it most preferable for photonic, electronic and sensor applications. It has been widely used in optical filters, optical modulators, beam deflectors and thin film photonic devices. It supports a low-loss transparency window covering from visible to mid-infrared wavelength regions. Modern day semiconductor fabrication techniques enhances refractive index contrast between the waveguide and substrate, and effectively reduces the size and hence low power consumption which is a major advantage with traditional LN devices [1-6].

It is well known that the physical properties of bulk crystals are very much different than those near the surface. Recently many researchers have evinced a lot of interesting the fabrication and design of thin film LN waveguides. LN is a uniaxial ferroelectric oxide material, with a negative
birefringence \((dn = -0.08)\) and remarkable optical anisotropy [7-11], large spontaneous polarization, [12-13] electro-optical and nonlinear optical activity [14-17]. For such work, the determination of refractive index profiles with depth assumes significant importance. Since optical waveguides are becoming increasingly thin, surface variations and near surface variations of refractive indices would have to be considered for evaluation of propagation parameters in such devices. The refractive index of any material is a function of the “Local” field experienced by the constituent ions [18]. The “Local” fields as experienced by ions on/near the surface of a dielectric medium ought to be different from those in the interior, thus one expects a refractive index variation near the surface of a material. In this paper, the variation of refractive indices \((n_x, n_y)\) and hence the birefringence near the surface of \(X\)-cut, \(Y\)-propagation LN open type waveguide and also the variation of \(n_x, n_y\) and the birefringence near the surface of \(Z\)-cut, \(X\)-propagation LN optical waveguide are reported.

2. Expressions for Refractive Indices – A Point Dipole Approach

Let us consider a \(LiNbO_3\) waveguide placed in an external electric field \(E_0\) of the incident light wave. Each atom of the waveguide becomes a dipole under the action of the electric field. Thus dipole moments could be attributed to these atoms and are treated as point dipoles at the appropriate lattice sites. The Lorentz fields are then evaluated at different lattice sites in the unit cell caused due to different atomic dipoles surrounding them by the method used by [18-23].

The dipole field at the origin due to dipoles of moment \(\mu_i\) at the position vectors \(r_i\) is given by

\[
E_{\text{dipoles}} = \sum_i \frac{3(\mu_i r_i) - r_i^2 \mu_i}{r_i^3}
\]

which can be resolved into

\[
E_{\text{dip}} = \mu_i \sum_i \frac{3x_i^2 - r_i^2}{r_i^3}
\]

where \(\mu_i\) is the component of the dipole moment of the \(i^{th}\) ion along the \(X\)-coordinate axis.

The local electric field “\(E_{\text{loc}}\)” at the site of an individual ion in a dielectric material is due to all the fields generated by sources external to the dielectric and also due to fields produced by all the ions in the material excluding the self-field of the ion itself [24-25] and is given by

\[
E_{\text{loc}} = E_0 + E_1 + E_2 + E_3
\]

Here \(E_0\) is the external field; \(E_1\) is the depolarization field due to the induced surface charges on the outer surface of the specimen; \(E_2\) is the Lorentz cavity field and \(E_3\) is the field due to all the dipoles inside the spherical cavity. We can write \(E = E_0 + E_1\), where \(E\) is the average macroscopic field. Hence

\[
E_{\text{loc}} = E + E_2 + E_3
\]

For a spherical cavity Lorentz has shown that

\[
E_2 = 4\pi P/3
\]

Here \(P\) is the Polarization vector.

The polarizability \(\alpha\) of an atom is defined in terms of the local electric field at the site of that atom as

\[
\mu = \alpha E_{\text{loc}}
\]

Here \(\mu\) is the dipole moment of the atom. The total polarizability \(\alpha\) can be written as a sum of four terms representing the most important contributions to the polarization [26]. Thus
\[ \alpha = \alpha_e + \alpha_i + \alpha_d + \alpha_s \]  

Here \( \alpha_e \), the electronic polarizability; \( \alpha_i \), the ionic polarizability; \( \alpha_d \), dipolar polarizability and \( \alpha_s \), the space charge polarizability. \( \alpha_s \) is the most important of all the four terms, being significant in the visible and in the ultra violet region. Consequently electronic polarization alone is considered in the present analysis.

Equation (6) can be written as \( \mu_j = \alpha \left( E + E_x + E_y \right) \) where the term in the bracket represents the local field at the site of the \( j \)th ion. Hence the polarization \( P \) can be written as

\[ P = \sum_j N_j \mu_j = \sum_j N_j \alpha_j E + \sum_j N_j \alpha_j E_z + \sum_j N_j \alpha_j E_{3j} \]  

Here \( N_j \) is the number of ions of the type \( j \) per unit volume. \( E_{3j} \) is the field due to all the dipoles within the cavity with the \( j \)th ion at the center of the cavity. Substituting for \( E_{2x} \) from equation (5), \( X \)-component of (8) is given by

\[ P_x = [\sum_j N_j \alpha_j E_x + (\sum_j N_j \alpha_j) K_x P_x + \sum_j N_j \alpha_j (\sum_i D_{ij} \mu_i)] \]  

where \( \sum_i D_{ij} = \sum \frac{3x^2 - y^2}{r_i^5} \) is a measure of the geometric anisotropy in the \( X \)-direction for all the \( i \)th ions with \( j \)th ion at the center. This may be called as the lattice anisotropy factor and \( K_x = 4\pi/3 \) is the depolarization factor for spherical cavity. The last term in the above equation can be further expanded as

\[ \sum_j N_j \alpha_j (\sum_i D_{ij} \mu_i) = [\sum_j N_j \alpha_j \sum_i D_{ij} \mu_i \sum_j N_j \alpha_j \sum_j D_{ij} \alpha_i K_x P_x + \sum_j N_j \alpha_j \sum_j D_{ij} \alpha_i E_{3ij}] \]  

Substituting equation (10) in (9) and rearranging, we have

\[ P_x = [\sum_j N_j \alpha_j E_x (1 + \sum_i D_{ij} \alpha_i) + \sum_j N_j \alpha_j K_x P_x (1 + \sum_i D_{ij} \alpha_i) + \sum_j N_j \alpha_j \sum_i D_{ij} \alpha_i E_{3ij}] \]  

Here \( E_{3ij} \) represents the dipole field of all the ions inside the cavity taking the \( i \)th ion as the origin. It can be expanded in exactly similar terms as in equation (10) viz \( E_{3ij} = \sum_i D_{ij} \alpha_i \). Hence the last term in equation (11) can be written as \( \sum_j N_j \alpha_j \sum_i D_{ij} \alpha_i \sum_j D_{ij} \alpha_i \). Since the magnitudes of \( \alpha \)’s are of the order of \( 10^{-24} \), the last term in the above expression comprises of the products of three \( \alpha \)’s and can be ignored with out any loss of accuracy. Hence equation (11) can be written as

\[ P_x = [\sum_j N_j \alpha_j E_x (1 + \sum_i D_{ij} \alpha_i) + \sum_j N_j \alpha_j K_x P_x (1 + \sum_i D_{ij} \alpha_i)] \]  

In a non-cubical crystal the dielectric response is described by the components of susceptibility tensor or of the dielectric constant tensor [18] as

\[ \chi_x = \frac{P_x}{E_x} = \frac{\varepsilon_x - 1}{4\pi} = \frac{n_x^2 - 1}{4\pi} \frac{-\sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i] K_x}{1 - \sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i]} \]  

Similarly the expressions for Refractive Indices for Electric vector vibrating along the crystallographic axes \( Y \) and \( Z \) are given by

\[ \frac{n_y^2 - 1}{4\pi} = \frac{-\sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i] K_y}{1 - \sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i]} \]  

\[ \frac{n_z^2 - 1}{4\pi} = \frac{-\sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i] K_z}{1 - \sum_j N_j \alpha_j [1 + \sum_i D_{ij} \alpha_i]} \]  

where \( K_x = K_y = K_z = 4\pi/3 \), since a spherical cavity is assumed.
From the equation (13) to equation (15) one can calculate, the refractive indices $n_o$ or $n_e$ by evaluating the lattice anisotropy factors $\Sigma D_j$ for various ions in the core of the waveguide along the principal crystallographic axes. The lattice anisotropy factors are shown in table 2. It is implied in these derivations that all the dipoles are aligned parallel to the applied external field direction.

Since Refractive Index is due to the dipole moments of the ions it can be expressed in terms of the polarizability of the ions and the effective local fields at the site of the ions. The ions near the surface and on the surface experience a different effective local field as compared to the ions well within the medium. This is because an ion near the surface sees a different environment when compared to an ion well within the lattice. There will be, consequently a variation in electrical field from ion to ion as we move from the surface to the interior of the crystal. Thus the geometric anisotropy factors $\Sigma D_j$’s would also vary from the surface to the interior and a gradation of Refractive Index from the surface to interior results. The variations in several properties have been discussed extensively in [27].

3. Results and discussion

An iterative programme is written in C++ to calculate $n_o$, $n_e$ and $n_r$ by using equation (13), equation (14) and equation (15) for the electric vector vibrating along the $X$, $Y$ and $Z$ axes by varying the values of polarizabilities $\alpha_i$ in small increments, one at a time. The local anisotropic factors $\Sigma D_j$’s are given in table 2. These values represent the ‘local field’ as seen by each of the species of Li, Nb and O. Finally polarizability values are found to be as shown table 3 to fit the calculated refractive indices with the experimental values [29-31].

Table 1. $n_o$ and $n_e$ representation for $X$, $Y$ and $Z$-cut waveguides along Cartesian Coordinates.

| Crystal Axis || Cartesian Axis | $n_x$ | $n_y$ | $n_z$ | Configuration Names |
|---------------|------------------|------|------|------|---------------------|
| c-axis || X-axis | $n_o$ | $n_o$ | $n_o$ | X-cut, $Y$-propagation |
| c-axis || Y-axis | $n_o$ | $n_o$ | $n_o$ | Y-cut, $X$-propagation |
| c-axis || Z-axis | $n_o$ | $n_o$ | $n_o$ | Z-cut, $X$-propagation |

Table 2. Lattice Anisotropy Factors $\left( \sum_i \sum_j D_{ij} / \sum_j D_{ij} \right) \times 10^{-24}$ cm$^3$ values obtained using PDA within the Core of LN Open Type Optical Waveguide at $\lambda=632.84$ nm along Cartesian $X$ and $Z$-axes.

| Effect On $\rightarrow$ | $\sum_i \sum_j D_{ij} = \sum_i \sum_j \frac{3z_i^2 - r_i^2}{r_i^2}$ | $\sum_i \sum_j D_{ij} = \sum_i \sum_j \frac{3z_i^2 - r_i^2}{r_i^2}$ |
|---------------|--------------------------|--------------------------|
| $L_i$ || $N_{bi}$ | $N_{bi}$ | $O_i$ | $L_i$ | $N_{bi}$ | $O_i$ |
| Li | -0.015020 | 0.039269 | 0.243708 | 0.030040 | -0.078538 | -0.487415 |
| Nb | 0.039269 | -0.015020 | 0.142383 | -0.078538 | 0.030040 | -0.284764 |
| O | 0.243708 | 0.142383 | -0.037617 | -0.487415 | -0.284764 | 0.075233 |
Table 3. Electronic Polarizability tuned values for various constituent ions of LN Open Type Optical Waveguide at \( \lambda = 6328 \text{ Å} \) within their limits of variation using PDA.

| Electronic Polarizability \( \alpha \times 10^{-24} \text{ cm}^3 \) | Refractive Indices | Birefringence \( (\Delta n = n_e - n_o) \) |
|-----------------------------------------------------------|------------------|-----------------|
| \( \alpha_{Li} = 0.029 \)                               | 2.28647          | -0.08407        |
| \( \alpha_{Nb} = 1.266562 \)                             | 2.28647          | -0.08407        |
| \( \alpha_{O} = 2.0044 \)                                | 2.2024           | 2.2024          |

3.1 Variation of Refractive Indices and birefringence near the Surface for an X-Cut, Y-propagation LN Open Type Optical Waveguide

In table 1, \( n_x \) and \( n_e \) directions for various crystal cuts in various Cartesian propagation directions are listed. For an open type X-cut LN waveguide, with the light propagation direction along Y-axis the \( c \)-axis of the unit cell coincides with the \( X \)-axis of the waveguide. The electric vector of light is considered to be along \( X \) and \( Z \) directions leading to evaluation of \( n_x \) and \( n_e \) in the waveguide.

Table 4. Lattice Anisotropy Factors \( (\sum_j \sum_l D_{Xj} / \sum_j \sum_l D_{Zj}) \times 10^{-24} \text{ cm}^3 \) for an X-Cut, Y-Propagation LN Waveguide for Various Depths at \( \lambda = 6328 \text{ Å} \).

| Effect On \( \rightarrow \) | \( \sum_j \sum_l D_{Xj} = \sum_j \sum_l \frac{3x_i^2 - r_i^2}{r_i^2} \) | \( \sum_j \sum_l D_{Zj} = \sum_j \sum_l \frac{3z_i^2 - r_i^2}{r_i^2} \) |
|-----------------------------|--------------------------------------------------|--------------------------------------------------|
| \( 0^{th} \) Unit Cell below the Surface (0Å - 13.863Å) | \( L_i \) 0.167806 0.213091 0.833129 -0.335599 -0.426215 -1.666211 |
| \( 1^{st} \) Unit Cell below the Surface (13.863Å - 27.276Å) | \( N_{B_{1}} \) 0.237875 0.167825 0.728313 -0.475750 -0.335658 -1.456623 |
| \( 2^{nd} \) Unit Cell below the Surface (27.276Å - 41.589Å) | \( O_{1} \) 0.838599 0.707280 1.746122 -1.677197 -1.414686 -3.492215 |
| \( 3^{rd} \) Unit Cell below the Surface (41.589Å - 55.452Å) | \( L_{i} \) 0.118769 0.180660 0.654985 -0.237538 -0.361321 -1.309969 |
| \( 4^{th} \) Unit Cell below the Surface (55.452Å - 69.315Å) | \( N_{B_{1}} \) 0.108048 0.059568 0.356452 -0.216095 -0.119136 -0.712900 |
| \( 5^{th} \) Unit Cell below the Surface (69.315Å - 83.178Å) | \( O_{1} \) 0.459865 0.376401 0.633936 -0.919730 -0.752800 -1.267872 |
In order to calculate the variation of the Refractive Indices near the surface, the waveguide is divided into regions of one-unit cell dimensions normal to the surface. As the Z-axis of the unit cell coincides with the X-axis of the waveguide. The 0th unit cell covers up to a depth of \(c = 13.863 \text{Å} \) 1st unit cell depth is of \(2c\), 2nd unit cell depth is of \(3c\), 3rd unit cell depth is of \(4c\), 4th unit cell depth of \(5c\) and 5th unit cell depth is of \(6c\) which represent the core part.

To calculate the refractive indices on the surface, a unit cell of LN touching the surface of the waveguide is considered. This unit cell is represented as 0th unit cell. The local field effects are within a radius of \(69.315 \text{Å} \) for different lattice sites with this position are evaluated. The centre is then shifted to 1st unit cell below the surface and local fields are evaluated. This procedure is continued to five times the lattice constant ‘c’ where the radius of the sphere of influence is \(69.315c^{2} \). At this position all the sphere of local field is totally within the core of the waveguide.

The local anisotropic factors \(\Sigma \Sigma D_{ij} 's\) are given in table 4. The values given in these tables represent the ‘local field’ as seen by each of the species of \(Li, Nb\) and \(O\) atoms. The values of Refractive Indices and Birefringence are given in table 6.

3.2 Variation of Refractive Indices near the Surface for a Z-Cut Open type LN Optical Waveguide

Here the cartesian Y-axis of the unit cell coincides with the Z-axis of the waveguide (See table-1). To calculate the variation of the Refractive Indices near the surface, the waveguide is divided into regions of one-unit cell dimensions normal to the surface. A unit cell of LN touching the surface of the waveguide is considered. This unit cell is represented as 0th unit cell. The local field effects at the different lattice sites with this position of the sphere are evaluated. The centre is then shifted to 1st unit cell below the surface and local fields are evaluated. This procedure is continued until the radius of the sphere of influence is \(69.315c^{2} \) which corresponds to 13.464 times the lattice constant ‘a’.

Table 5a. Lattice Anisotropy Factors \((\Sigma \Sigma_{i} D_{xy}/\Sigma \Sigma_{i} D_{xw}) \times 10^{24} \text{cm}^{3}\) for Z-Cut, Y-Propagation LN Waveguide at various Depths at \(\lambda=6328 \text{Å}\).

| Effect On | Effect due to ↓ |
|-----------|----------------|
| \(L_{i}\) | \(N_{bi}\) | \(O_{i}\) | \(L_{i}\) | \(N_{bi}\) | \(O_{i}\) |
| 0th Unit Cell below the Surface (0Å – 5.148Å) |
| \(L_{i}\) | -0.214217 | -0.266957 | -0.687163 | 0.169323 | 0.200322 | 0.310994 |
| \(N_{bi}\) | -0.214878 | -0.214217 | -0.597222 | 0.199166 | 0.169233 | 0.278753 |
| \(O_{i}\) | -0.234367 | -0.473435 | -2.018370 | 0.126185 | 0.062336 | 1.594724 |
| 1st Unit Cell below the Surface (5.148Å – 10.296Å) |
| \(L_{i}\) | -0.267439 | -0.215060 | -0.499495 | 0.231201 | 0.124942 | 0.108205 |
| \(N_{bi}\) | -0.215782 | -0.267439 | -0.597635 | 0.125968 | 0.231201 | 0.306228 |
| \(O_{i}\) | -0.544576 | -0.631674 | -2.312632 | 0.145697 | 0.330569 | 1.890893 |
| 2nd Unit Cell below the Surface (10.296Å – 15.444Å) |
| \(L_{i}\) | -0.240424 | -0.185979 | -0.414222 | 0.210388 | 0.101457 | 0.039168 |
| \(N_{bi}\) | -0.185833 | -0.240424 | -0.515274 | 0.101425 | 0.210388 | 0.241214 |
| \(O_{i}\) | -0.451555 | -0.552377 | -2.065591 | 0.068948 | 0.270891 | 1.697242 |
| 3rd Unit Cell below the Surface (15.444Å – 20.592Å) |
| Effect On Due to ↓ | \( \sum_i \sum_j D_{ij} = \sum_i \sum_j \frac{3x^2 - r^2}{r^2} \) | \( \frac{\sum_i \sum_j D_{ij}}{\sum_i \sum_j D_{ij}} \times 10^{-24} \text{cm}^3 \) |
|----------------|--------------------------------|-----------------|
| \( L_i \)     | -0.160317 -0.104380 -0.167891 | 0.146581 0.301896 |
| \( N_b \)     | -0.106171 -0.167017 -0.278000 | 0.037692 0.146581 |
| \( O_i \)     | -0.210317 -0.311307 -1.348175 | 0.078187 1.307783 |
| 4th Unit Cell below the Surface (20.592A\(\text{o}\) – 25.740A\(\text{o}\))
| \( L_i \)     | -0.160317 -0.104380 -0.167891 | 0.146581 0.301896 |
| \( N_b \)     | -0.106171 -0.167017 -0.278000 | 0.037692 0.146581 |
| \( O_i \)     | -0.210317 -0.311307 -1.348175 | 0.078187 1.307783 |
| 5th Unit Cell below the Surface (25.740A\(\text{o}\) – 30.888A\(\text{o}\))
| \( L_i \)     | -0.136449 -0.081880 -0.104928 | 0.127141 0.208274 |
| \( N_b \)     | -0.081385 -0.136449 -0.206055 | 0.018370 0.140190 |
| \( O_i \)     | -0.136443 -0.237438 -1.129561 | 0.078187 1.234324 |
| 6th Unit Cell below the Surface (30.888A\(\text{o}\) – 36.036A\(\text{o}\))
| \( L_i \)     | -0.113645 -0.059066 -0.067047 | 0.108834 0.208274 |
| \( N_b \)     | -0.059066 -0.113645 -0.138851 | 0.108834 0.059744 |
| \( O_i \)     | -0.067047 -0.168037 -0.237813 | 0.078477 0.140190 |
| 7th Unit Cell below the Surface (36.036A\(\text{o}\) – 41.184A\(\text{o}\))
| \( L_i \)     | -0.092674 -0.038061 -0.002819 | 0.092096 0.208274 |
| \( N_b \)     | -0.038061 -0.092674 -0.077157 | 0.092096 -0.109080 |
| \( O_i \)     | -0.002819 -0.103814 -0.735932 | -0.087816 0.633916 |
| 8th Unit Cell below the Surface (41.184A\(\text{o}\) – 46.332A\(\text{o}\))
| \( L_i \)     | -0.073688 -0.019125 0.055538 | 0.092096 -0.109080 |
| \( N_b \)     | -0.019079 -0.073688 -0.021637 | 0.092096 -0.109080 |
| \( O_i \)     | 0.055538 -0.045476 -0.565071 | -0.306458 0.784747 |
| 9th Unit Cell below the Surface (46.332A\(\text{o}\) – 51.480A\(\text{o}\))
| \( L_i \)     | -0.056959 -0.002368 0.128098 | 0.092096 -0.355909 |
| \( N_b \)     | -0.002325 -0.056959 0.026960 | 0.092096 -0.355909 |
| \( O_i \)     | 0.107290 0.006279 -0.414449 | 0.078477 0.633916 |
| 10th Unit Cell below the Surface (51.480A\(\text{o}\) – 56.628A\(\text{o}\))
| \( L_i \)     | -0.042684 0.011853 0.169139 | 0.052110 -0.427639 |
| \( N_b \)     | 0.011900 -0.042684 0.067945 | 0.056609 0.052110 |
| \( O_i \)     | 0.151767 0.050756 -0.286205 | 0.274079 0.376741 |
| 11th Unit Cell below the Surface (51.480A\(\text{o}\) – 61.776A\(\text{o}\))
| \( L_i \)     | 0.146875 -0.009749 0.035769 | 0.056609 0.052110 |
| \( N_b \)     | 0.023413 -0.031102 0.106858 | 0.065862 0.042847 |
| \( O_i \)     | 0.188220 -0.087203 -0.182577 | 0.240531 0.191125 |
| 12th Unit Cell below the Surface (61.776A\(\text{o}\) – 66.924A\(\text{o}\))

Upto a Depth of 69.315A\(\text{o}\) below the Surface (66.924A\(\text{o}\) – 69.315A\(\text{o}\))
The local anisotropic factors ‘$\Sigma D$’ are given in table 5a and table 5b. The values given in these tables represent the ‘local field’ as seen by each of the species of Li, Nb and O atoms. The values of Refractive Indices and Birefringence are given in table 7.

**Table 6.** $n_x, n_y$ and $\Delta n$ variation near the surface for $X$-cut, $Y$-propagation waveguide at $\lambda=6328\text{A}$.  

| Depth (in A) | Refractive Indices $n_{x}$ | Refractive Indices $n_{y}$ | Birefringence $(\Delta n = n_{x} - n_{y})$ |
|-------------|-----------------------------|-----------------------------|----------------------------------|
| $0 \times c = 0$ | 2.969637 1.484915 | -1.484722 |
| $1 \times c = 13.863$ | 2.710879 1.670473 | -1.040406 |
| $2 \times c = 27.726$ | 2.504855 1.877748 | -0.627107 |
| $3 \times c = 41.589$ | 2.368434 2.063002 | -0.305432 |
| $4 \times c = 55.452$ | 2.298410 2.180441 | -0.117969 |
| $5 \times c = 69.315$ | 2.286470 2.202400 | -0.084070 |

*a = 5.148 A° and *c = 13.863 A° are the lattice constants along $a$ and $c$-axis.

**Table 7.** $n_x, n_y$ and $\Delta n$ variation near the surface for $Z$-cut, $X$-propagation LN waveguide at $\lambda=6328\text{A}$. 

| Depth (in A) | Refractive Indices $n_{x}$ | Refractive Indices $n_{y}$ | Birefringence $(\Delta n = n_{x} - n_{y})$ |
|-------------|-----------------------------|-----------------------------|----------------------------------|
| $0 \times a = 0$ | 1.804680 2.700559 | 0.895879 |
| $1 \times a = 5.148$ | 1.749574 2.851358 | 1.101784 |
| $2 \times a = 10.296$ | 1.797415 2.764275 | 0.966860 |
| $3 \times a = 15.444$ | 1.847415 2.680592 | 0.833177 |
| $4 \times a = 20.592$ | 1.898013 2.604278 | 0.706265 |
| $5 \times a = 25.740$ | 1.948684 2.535160 | 0.586476 |
| $6 \times a = 30.888$ | 1.998825 2.472966 | 0.474141 |
| $7 \times a = 36.036$ | 2.047786 2.417391 | 0.369605 |
| $8 \times a = 41.184$ | 2.094758 2.368377 | 0.273619 |
| $9 \times a = 46.332$ | 2.138903 2.325618 | 0.186715 |
| $10 \times a = 51.480$ | 2.179210 2.289164 | 0.109954 |
| $11 \times a = 56.628$ | 2.214634 2.258932 | 0.044298 |
| $12 \times a = 61.776$ | 2.244056 2.235042 | -0.009014 |
| $13 \times a = 66.924$ | 2.266427 2.217578 | -0.048849 |
| $5 \times c = 69.315$ | 2.286470 2.202400 | -0.084070 |

*a = 5.148 A° and *c = 13.863 A° are the lattice constants along $a$ and $c$-axis.
along crystallographic $X$ and $Z$-axes respectively.

4. Summary and Conclusions

The calculations are carried out for waveguide at wavelength 632.8 nm. $n_0$ is found to increase from 1.484915 at the surface to 2.2024 in the interior, whereas $n_e$ is found to decrease from 2.969637 at the surface to 2.2864 in the interior of the waveguide. All the variations take place within a distance of 69.315 Å, from the surface. The opposite behaviour in the variation of $n_0$ and $n_e$ at the surface of the $X$–cut, $Y$–propagation and $Z$–cut, $X$–propagation waveguides are primarily due to the dipole orientation and their relative distributions in the lattice being different for the two directions of the electric vectors of light as is evident from the values.
The refractive index variation near the surface as indicated in these calculations must be considered in the analysis of all such optical waveguides and in the studies involving the propagation mechanisms of light through such integrated optical devices.

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