Inverse Design of Lithium Niobate Modulators Using a Genetic Algorithm

Ademar Muraro Júnior¹, Angelo Passaro¹, Airam Jonatas Pretó², Stephan Stephany²

Abstract - Integrated optics devices are currently being employed to increase transmission bandwidth in telecommunication equipment. Particularly, electrooptical modulators are among the most important devices, since they provide external modulation in fiber-optics transmission systems. The lithium niobate modulators are compatible with the bandwidth requirements of these systems and minimize fiber dispersion. The investigation of materials, components and physical configuration of integrated optics devices present characteristic aspects that not always allow an analytical evaluation of the device performance, requiring the manufacturing of several prototypes for experimental evaluation. This lengthens the design, evaluation and optimization cycle. The use of a software to model the electrooptic behavior of these devices significantly reduces their development cost and time. For a given choice of device materials and configuration, the software would allow to analyze the performance of the device. However, such software must be able to model materials that are anisotropic and non-homogeneous, and devices that present complex geometric configurations. This work presents the optimization of some design parameters of a lithium niobate modulator using a genetic algorithm to iteratively refine candidate set of parameters. Each of these candidate solutions is evaluated by applying the Finite Element Method. Numerical results show that the genetic algorithm is able to optimize design parameters of the lithium niobate modulator. Test cases include optimization of single and multiple parameters of the modulator. The set of characteristics include the half wave voltage, the electrode characteristic impedance, and the resulting bandwidth of the device.

Keywords - Electrooptical modulators, optimization, genetic algorithms, finite element methods.

1. Introduction

The demand for telecommunication services and bandwidth has increased since the past decade. Integrated optic devices are currently being employed to increase transmission bandwidth and electrooptical modulators are among the most important devices, since they can provide external modulation, one of the main requests in fiber optics communication systems. Particularly, the lithium niobate modulators are compatible with the bandwidth requirements of these systems and minimize fiber dispersion [1]. Additionally lithium niobate presents advantages in comparison with other electrooptical materials [2]. The investigation of materials, components and physical configuration of integrated optic devices presents aspects that not always allow an analytical evaluation of the device performance, requiring the manufacturing of several prototypes for experimental evaluation. This lengthens the design, evaluation and optimization cycle. The use of a computational model for simulate the electrooptic behavior of these devices significantly reduces their development cost and time. For a given choice of materials and configuration, the software would allow to analyze the performance of the device.

Several heuristics have been used in optimization problems for different applications [3]. Stochastic methods are often employed due to the easy of implementation and good trade-off between the quality of the solution and processing time [4]. In the case of the more complex multiobjective problems, specific optimization techniques were developed [5][6][7][8][9][10]. In the last years, standard optimization methods have been enhanced and present better performance. Considering the design optimization of electromagnetic devices, that is similar to the optimization of optical devices, several approaches have been proposed, using stochastic methods, hybrid methods (that combine a deterministic and a stochastic method, for instance) and multiobjective methods [11][12][13][14].

In the optimization process, each candidate solution must be evaluated. In the case of electrooptical modulators, most authors use the Finite Element Method, the Beam Propagation Methods or the Line Method to solve the associated problem [15][16][17] in order to analyze or characterize the device. The performance of the optimization depends on the design experience. Only a few works describe the use of stochastic methods for the design optimization of devices, but being restrained to only the optimization of one design parameter, as for example the half wave voltage $\frac{\pi}{f}$ [18].

In this work, the computational analysis is performed by using a numerical optimization technique, in order to explore the effect of some geometric parameters of the coplanar waveguide on the performance of the modulator. A genetic algorithm (GA) is used for the design optimization of the electrooptical modulator and the finite-element method (FEM) is applied on each candidate solution generated by GA to study both the optical properties of Ti:LiNbO$_3$ waveguide and the quasi-static propagation transverse electromagnetic (TEM) modes of the coplanar waveguides (CPW).

To minimize the computational execution time, the optimization software was implemented in order to be executed in a distributed memory parallel environment. This environment is composed by a cluster of PC's microcomputers interconnected by a switch Fast-Ethernet network. The parallelization of the software employed the the MPICH implementation[19] of the Message Passing Interface communication library (MPI).

In section 2, the parameters often used as figure of merit of an electrooptical modulator are reviewed. The FEM simulation technique used to solve the optical and electric fields is shown in section 3. Section 4 describes, briefly, the genetic algorithms. Section 5 presents the optimization approach used in this work. The results of the optimization are discussed in section 6, and section 7 presents the main conclusions and the future work associated to the analysis and optimization of this sort of devices.
2. Mach-Zehnder Modulators on Lithium Niobate

The cross section of a Mach-Zehnder modulator with CPW is presented in Figure 1. In the figure, \( t_b \) is the thickness of the buffer layer, \( T_e \) is the electrode thickness, \( G \) is the gap between the hot electrode and the ground electrode and \( W_h \) is the width of the hot electrode.

![Cross section of the Mach-Zehnder modulator](image)

The modulator can be characterized by analysis of the same electrical parameters such as: the characteristic impedance \( (Z_c) \), the half-wave voltage \( (V_{\frac{1}{2}}) \), the effective index of the transverse electromagnetic wave \( (N_{eq}) \) and the bandwidth \( (\Delta f) \). The definitions of these parameters are:

\[
Z_c = \frac{1}{c} \sqrt{\frac{1}{C_1 C}}
\]

\[
V_{\frac{1}{2}} L = \frac{\lambda_0 G}{n_{le} r_3} |\Gamma| |\Gamma|_1
\]

\[
N_{eq} = \sqrt{\frac{C}{C_1}}
\]

\[
\Delta f L = \frac{4.14 c}{\pi \sqrt{|\varepsilon_{eff} - n_{eff}|}}
\]

In the equations (1)-(4), \( C \) and \( C_1 \) are the capacitance per unit length of the CPW calculated with the dielectric materials and with the materials replaced by vacuum, respectively, \( c \) is the free-space light velocity, \( n_{le} \) is the effective index of the optical wave, \( V \) is the applied voltage, \( L \) is the length of CPW electrodes, \( \lambda_0 \) is the free-space optical wavelength, \( n_{eq} \) is the extraordinary refractive index of the substrate, \( r_3 \) is the pertinent electrooptic coefficient and \( \Gamma \) is the overlap factor between the electric field of the (optical wave) lightwave and the electric field induced by the electrodes. For x-cut Mach-Zehnder modulators, the optical waveguides are in the middle of the gap \( G \) and the overlap factor is equal in both waveguides \( |\Gamma| = |\Gamma|_1 = |\Gamma|_2 \). The overlap factor for each waveguide is defined as:

\[
\Gamma = \frac{G}{\pi} \int E_{mp}^2(x,y)E_{el}^2(x,y) dx dy
\]

where \( E_{mp} \) is the optical modal electric field and \( E_{el} \) is the electric field of the electrode structure (TEM wave and \( E_x \) component for x-cut configuration).

The optical waveguides used in this sort of devices are built by diffusing ions (usually Ti, or protons) in a dielectric substrate. One of the most used substrate in integrated optical circuits is the LiNbO\(_3\), because it presents appropriate optical and mechanical properties. In the fabrication process, a diffused channel, in which the refractive index varies continuously, is produced.

3. Finite Element Model

The finite element method (FEM) is based on the minimization of a functional whose solution is equivalent to the original differential equation. An approximated solution for a set of differential equations can be obtained by applying the Weighted Residual Method (WRM) or by applying variational principles. The finite element formulations adopted in the computations performed in this work were used in previous works [20] and are briefly presented in the next sub-sections.

3.1 Propagation in the CPW

In this work, \( E_z \) is computed by the FEM in the quasi-static approximation (TEM modes). The TEM modes are related to the solutions of the Laplace equation for the electric potential \( \phi \):

\[
\nabla (\varepsilon \nabla \phi) = 0
\]
where the diagonal relative permittivity tensor is given by:

$$\varepsilon_r = \begin{bmatrix} \varepsilon_{xx} & 0 \\ 0 & \varepsilon_{yy} \end{bmatrix}$$

(7)

The FEM applied to (6) yields the matrix equation:

$$[S][\phi]^T = [b]^T$$

(8)

where:

$$[S] = \int_{\Omega} \left( \varepsilon_\sigma \frac{\partial [N]^T}{\partial x} \frac{\partial [N]}{\partial x} + \varepsilon_\varphi \frac{\partial [N]^T}{\partial y} \frac{\partial [N]}{\partial y} \right) dx dy$$

$$\phi = [N]_i[\phi]^T$$

and

$$E = -\nabla \phi$$

{ } represents a row matrix, { }^T stands for a transposed matrix and \( [N] \) represents a complete set of base functions for the used finite elements.

3.2 Propagation in anisotropic optical waveguides

From an electromagnetic point of view, the optical waveguides considered in this work do not present well-defined borders, which means that the electromagnetic fields in the direction perpendicular to the light propagation can extend to very large dimensions. The guiding effect is a consequence of the difference in the refractive index between the diffused waveguide and the substrate.

In metallic waveguides filled with dielectric material only pure TE (transverse electric) and TM (transverse magnetic) modes are present. However, in optical waveguides, electromagnetic fields with different configurations propagate and a different classification must be used. In the discussion that follows, the z-axis coincides with the direction of propagation of the optical wave. For short wavelengths and small refractive index differences (weak guidance), the transversal electric field is parallel to one of the transversal axis. If the electric field is parallel to the y-axis, the propagation modes are named \( E^z \) and if it is parallel to the x-axis the propagation modes are named \( E^x \).

The \( E^x \) modes can be represented by a quasi-TE approximation, in which \( E_y = 0 \) and the solutions for the wave equation are obtained from the \( E_z \) component of the electric field. In the same way, the representation of the \( E^y \) mode is obtained by the quasi-TM approximation: the component \( H_x = 0 \) and the solutions are obtained from the \( H_y \) component of the magnetic field [21].

In order to obtain the wave equation for the \( E^x \) and \( E^y \) modes, considering a dielectric material that is anisotropic, non-homogeneous, presents no losses, relative magnetic permeability equal to 1, and the relative permittivity tensor given by:

$$\varepsilon_r = \begin{bmatrix} n_x^2(x, y) & 0 & 0 \\ 0 & n_y^2(x, y) & 0 \\ 0 & 0 & n_z^2(x, y) \end{bmatrix}$$

(10)

In these conditions, the scalar Helmholtz equation for \( E^x \) modes is given by:

$$n_x^2 \frac{\partial}{\partial x} \left( \frac{1}{n_x^2} \frac{\partial (n_x^2 E_x)}{\partial x} + \frac{\partial (n_y^2 E_y)}{\partial y} + n_y^2 \frac{\partial^2 E_y}{\partial y^2} \right) + k_0^2 n_x^2 n_y^2 E_x = n_x^2 \beta^2 E_x$$

(11)

where \( \beta \) is the propagation constant and \( k_0^2 = \omega^2 \mu_0 \varepsilon_0 \) is the wave number in vacuum. These parameters define the effective refractive index of the optical wave: \( n_{eff} = \beta / k_0 \).

For the \( E^y \) modes the wave equation is:

$$n_y^2 \frac{\partial^2 H_y}{\partial x^2} + n_x^2 \frac{\partial}{\partial y} \left( \frac{1}{n_x^2} \frac{\partial H_x}{\partial y} \right) + n_y^2 n_x^2 H_x = \beta^2 H_x$$

(12)

The FEM formulation is obtained by applying the Weighted Residual Method allied to the Galerkin approximation on the equations (11) and (12), resulting the follow matricial equation:

$$[F][\phi]^T - k_x^2[M][\phi]^T = [0]^T$$

(13)

The matrices for each finite element are given by:
\[ [M] = \int_\alpha A k_0^2 |N| \frac{\partial}{\partial x} |N| \, dx \, dy, \]

\[ |F| = |F_1| - |F_2| \]

where the parameter \( A \) and the matrices \([F_1]\) and \([F_2]\) depend on the propagation mode considered. For \( E^2 \) modes, \( A = n_e^2 \) and the matrices are:

\[ [F_1] = \int_\alpha \left( k_0^2 n_e^2 |N|^T \frac{\partial |N|}{\partial x} \right) dx \, dy \]

\[ - \int_\alpha n_e^2 \frac{\partial|N|^T}{\partial x} \frac{\partial|N|}{\partial x} \, dx \, dy \]

\[ [F_2] = \int_\alpha \delta_e \frac{\partial n_e^2}{\partial x} \frac{\partial |N|^T}{\partial x} |N|^T \frac{\partial |N|}{\partial x} \, dx \, dy \]

For the \( E^2 \) modes, \( A = 1 \) and:

\[ [F_1] = \int_\alpha \left( k_0^2 n_e^2 |N|^T \frac{\partial |N|}{\partial x} \right) dx \, dy \]

\[ - \int_\alpha n_e^2 g_e \frac{\partial |N|^T}{\partial x} \frac{\partial |N|}{\partial x} \, dx \, dy \]

\[ [F_2] = \int_\alpha \left( \delta_e g_e \delta_e \frac{\partial n_e^2}{\partial x} \frac{\partial |N|^T}{\partial x} + \delta_e n_e^2 \frac{\partial|N|^T}{\partial x} \frac{\partial |N|}{\partial x} \right) \, dx \, dy \]

In both propagation modes, \( g_e = 1/n_e \). The parameters \( \delta_e \) and \( \delta_e \) assume either the value 1 for material in which the refractive indexes \( n_e \) are homogenous, or zero for homogenous materials. The matrix \([F_2]\) is sparse and non-symmetric, due to the presence of the partial derivatives on the refractive index.

4. Genetic Algorithms

The genetic algorithms [22], which mimics survival of the fittest among competing organisms, have seen wide application in recent years [23]. The algorithm used in this study is standard in most respects. An initial population of \( N_p \) chromosomes (individuals) is constructed randomly, with each group of bits in a chromosome corresponding to a geometric parameter. The geometric model of a modulator is then configured according to each chromosome and the fitness of each configuration is evaluated by computing the characteristic electric parameter. A selection process follows, during which a new population of size \( N_p \) is created. During selection, individuals are chosen from the old population with a probability equal to the ratio of the individual fitness to the total fitness of the old population. Regardless of the result, the individuals with the highest fitness values are selected to guarantee their genetic information will be passed along to the next generation. This scheme is known as elitism. After selection, individuals are paired off as parents and crossed over, each with a crossover probability. Each time crossover occurs, the chromosomes are split at a random bit location and their partial bit strings (all bits before the random bit) are swapped between the parents. Following crossover, a mutation is performed by negating each bit on each chromosome with a mutation probability. The fitness of each resulting individuals is evaluated, and the process is repeated for a specific number of generations or until that a convergence criterion is reached.

5. Optimization Approach

There are two main choices in a design optimization process: the analysis tool and the optimization/search algorithm. The optimization design is an iterative process and candidate solutions are successively generated by the optimization algorithm and evaluated by the analysis tool.

In this work, the GA realize the search operation and the FEM carries out the analysis. Figure 2 presents a diagram of the optimization process used in this work.

The size of the GA initial population is 60 individuals. The individuals of the initial population are generated randomly. Two design parameters (gap and thickness of the electrodes) are coded into a 20 bit string segments using binary coding. These segments are appended one after the other to form a chromosome. The roulette wheel technique is used for the reproduction operator, with one-point crossover. The occurrence probability for the crossover is set to 0.8 and for mutation is set for 0.05. Elitism is applied using 1 or 4 individuals.
5.1. Optimization parameters
The GA works with the values of electrode cross-sectional parameters (gap $G$, buffer thickness $T_b$, electrode thickness $T_e$ and width $W$). The boundaries parameters used in the optimization process are in the range that can be manufactured by the current processing technology (thickness up to 30 $\mu$m and 1 $\mu$m to electrode and buffer, respectively) [18].

![Flowchart of the design optimization process.](image)

These parameters are summarized as:

- $10 \mu$m $\leq W \leq 30 \mu$m
- $5 \mu$m $\leq G \leq 25 \mu$m
- $20 \mu$m $\leq T_e \leq 30 \mu$m
- $0.5 \mu$m $\leq T_b \leq 1 \mu$m

In all optimization cases, it was assumed a value of $n_{eff} = 2.1419$ for the effective index of the optical wave.

6. Optimization Results
In order to test the proposed design optimization method, only two parameters of the modulator were optimized, to obtain the better characteristic impedance ($Z_c$). The primary objective of the optimization is to find a modulator configuration that offers a $Z_c$ as close as the impedance of commercial microwave sources, namely 50 $\Omega$. The result is shown in Figure 3.

Although none of the several configurations of the geometric model tested by the optimization process reached the ideal impedance ($Z_c = 50 \Omega$), the convergence of the process was fast (18th generation for elitism of 4 individuals and 34th for elitism of 1 individual).

![Change of fitness over generations for characteristic impedance ($Z_c$) of the modulator.](image)

With the implementation of the optimization process established, it was used to explore other electrical parameters, such as the half-wave voltage ($V_{\pi}$), and the effective index of the transverse electromagnetic wave ($n_{eff}$). The best results that were obtained by the optimization process are present in Tables 1, 2 and 3.
I n  th i s  w o r k ,  a  d e s i g n  o p t i m i z a t i o n  m e t h o d  w a s  p r o p o s e d  f o r  M a c h - Z e h n d e r  m o d u l a t o r s .  T h e  F i n i t e  E l e m e n t  M e t h o d  w a s  e m p l o y e d  b e t w e e n  t h e  m o d u l a t o r  a n d  t h e  m i c r o w a v e  s o u r c e , r e s u l t i n g  t h e  n e e d  f o r  a  m o r e  p o w e r f u l  s o u r c e  t o  m o d u l a t e  t h e  s i g n a l .

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Table 1. Optimization result for $Z_e$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrode gap ($G$)</td>
<td>25 µm</td>
</tr>
<tr>
<td>Electrode thickness ($T_e$)</td>
<td>20 µm</td>
</tr>
<tr>
<td>Electrode width ($W_{ge}$)</td>
<td>10 µm</td>
</tr>
<tr>
<td>Buffer layer thickness ($T_b$)</td>
<td>0.5 µm</td>
</tr>
<tr>
<td>$V_e$</td>
<td>12.4182 V.cm</td>
</tr>
<tr>
<td>$N_{ef}$</td>
<td>2.52025</td>
</tr>
</tbody>
</table>

Table 2. Optimization result for $V_e$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrode gap ($G$)</td>
<td>5 µm</td>
</tr>
<tr>
<td>Electrode thickness ($T_e$)</td>
<td>30 µm</td>
</tr>
<tr>
<td>Electrode width ($W_{ge}$)</td>
<td>30 µm</td>
</tr>
<tr>
<td>Buffer layer thickness ($T_b$)</td>
<td>0.5 µm</td>
</tr>
<tr>
<td>$Z_e$</td>
<td>12.0506 Ω</td>
</tr>
<tr>
<td>$N_{ef}$</td>
<td>1.8236</td>
</tr>
</tbody>
</table>

Table 3. Optimization result for $N_{ef}$

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Electrode gap ($G$)</td>
<td>11 µm</td>
</tr>
<tr>
<td>Electrode thickness ($T_e$)</td>
<td>29 µm</td>
</tr>
<tr>
<td>Electrode width ($W_{ge}$)</td>
<td>24 µm</td>
</tr>
<tr>
<td>Buffer layer thickness ($T_b$)</td>
<td>0.5 µm</td>
</tr>
<tr>
<td>$Z_e$</td>
<td>18.7686 Ω</td>
</tr>
<tr>
<td>$V_e$</td>
<td>6.17824 V.cm</td>
</tr>
</tbody>
</table>

As can be seen from Table 3, the optimization process for the effective index $N_{ef}$ was quite significative, reaching to 0.2% of the intended value $n_{ef}$, but this optimum configuration is not suitable for the optimization criterion for $Z_e$. The best result obtained for the $V_e$ voltage (Table 2) also presents an impedance value far from the ideal one.

From these results, one can see that for this type of device, the optimum configuration obtained for one parameter is not the best for the others. This behavior can be seen in Figure 4, where the results obtained varying only the electrode thickness are shown. As the values of $N_{ef}$ and $n_{ef}$ gets closer, improving the bandwidth $\Delta f$ (Eq. (4)), the value of $Z_e$ decreases. This leads to a phase mismatch between the modulator and the microwave source, resulting the need for a more powerful source to modulate the signal.

The same behavior can be seen in Figure 5, which shows an analysis of the influence to the electrode gap. An increasing of the $Z_e$ value leading to a better impedance matching increases the value of $V_e$ voltage, which should be the lowest as possible.

7. Conclusion
In this work, a design optimization method was proposed for Mach-Zehnder modulators. The Finite Element Method was employed to model the device and to analyze the performance of the electrooptical modulator for each candidate solution. A Genetic Algorithm performed the optimization. In a first approach, the optimization process was applied by changing two parameters of the modulator since it is difficult to model all the parameters of a real device. Results show the feasibility of the proposed approach. The use of parallel computing was required in order to obtain results in a feasible time. The next step would be to perform a multiobjective optimization, including the characteristic impedance, the half-wave voltage and the effective index of the electromagnetic wave.

The current FEM model takes into account the parameters that are related to the electrical behavior of the modulator, but a more precise approach would require the inclusion of parameters of the optical wave guide, for instance the duration and temperature of the ion diffusion process that have a influence in the dimensions of this waveguide. Therefore, a full multiobjective optimization of this kind of devices will require a more complete and accurate model and consequently more processing time.
Figure 4. Variation of impedance characteristic ($Z_c$) and effective index of the transverse electromagnetic wave ($N_{eff}$) with thickness electrode ($Te$).

Figure 5. Variation of impedance characteristic ($Z_c$) and half-wave voltage ($V_{ph}$) with thickness gap ($G$).

8. References
15. Anwar, N. et al. The Effect of Fabrication Parameters on a Ridge Mach-Zehnder Interferometric (MZI) Modulator. Journal of