Finite Element Modelling of Liquid Crystal Orientation and Its Applications in a Tunable Bimodal Periodic Waveguide

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Liquid Crystal (LC) materials are promising candidates to be implemented in reprogrammable integrated photonics due to their capability to electronically modulate their effective refractive index. However, the performance of these materials is highly dependent on the device features, surface alignment, or electrode geometry. In this work, we present a simulation framework that comprises both the 3D LC orientation modelling and the 3D FDTD optical simulation. These two types of simulations have been implemented for a bimodal periodic waveguide, contributing to a better comprehension of the optical performance implications associated with the application of LC claddings.

Introduction

Programmable photonic circuits are constructed as a large tunable interferometric circuit with electro-optic phase shifters such as waveguide heaters, MEMS or Liquid Crystal (LC) actuators [1], [2]. The large birefringence of LC results in the possibility to locally tune the effective index of propagating modes in integrated photonic devices when an electrical field is applied. In [3] the localized deposition of LC on a chip surface is demonstrated, where silicon side-rail electrodes are used to apply a confined electric field to build an electro-optic phase shifter.

Usually, interferometric devices are constructed as an on-chip Mach-Zehnder-Interferometer (MZI) circuit with an electro-optic phase shifter embedded in the arms [1]. In [4] however, a 1D photonic crystal is presented that condenses the MZI circuit to one single component. The device operates using two propagating modes with different propagation constants. The wavelength dependent phase difference between these two modes results in an interference pattern in the transmission spectrum, where the peaks can be shifted by tuning the cladding refractive index. In this work, we simulate how an LC cladding with electrical fields using silicon electrodes (like [3]) would shift the wavelengths where destructive interferences occur.

The simulation process involves the use of multiple tools, starting from an initial design built in GID (https://www.gidsimulation.com/) where a triangular mesh is used to model the LC volume, which is shown in Figure 2b. This mesh is imported into a Finite Element Method (FEM) model implemented in Matlab where the LC orientations for different voltages are computed, providing the corresponding Q-tensor distributions [5]. The Q-tensor is a mathematical object that contains the director information and can be converted into LC orientation unit vectors (n_x, n_y, n_z). The director distribution is imported into a

Finite Difference Time Domain (FDTD) solver (*Ansys Lumerical*) to carry out the optical 3D simulations.

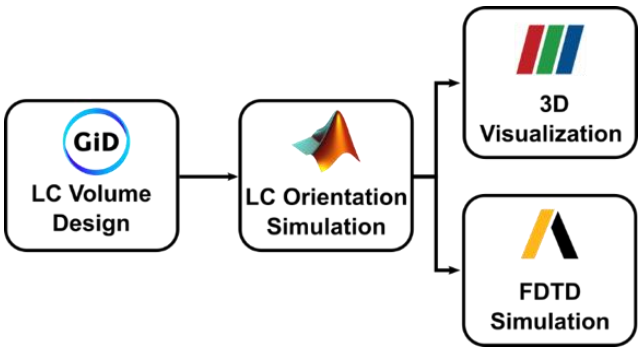

Figure 1: Simulations overview block diagram.

Finite Element Simulation of Liquid Crystal Orientation

The cross sections of simulated LC unit cell volume are shown in Figure 2a with the implementation of the boundary conditions. We use a triangular mesh of tetrahedra (see Figure 2b) of the unit cell to minimize the Laundau-de-Gennes energy functional in each element for a given voltage with a FEM calculation. This results in the local Q-tensor of each element of the mesh which can be transformed into the director components, i.e., (n_x,n_y,n_z), resulting in the director distribution [6]. The simulated LC distributions of the cross-section of the unit cell are shown in Figure 2c,d, corresponding to an applied voltage of 0 V and 10 V, visualizing the director distribution in this plane.

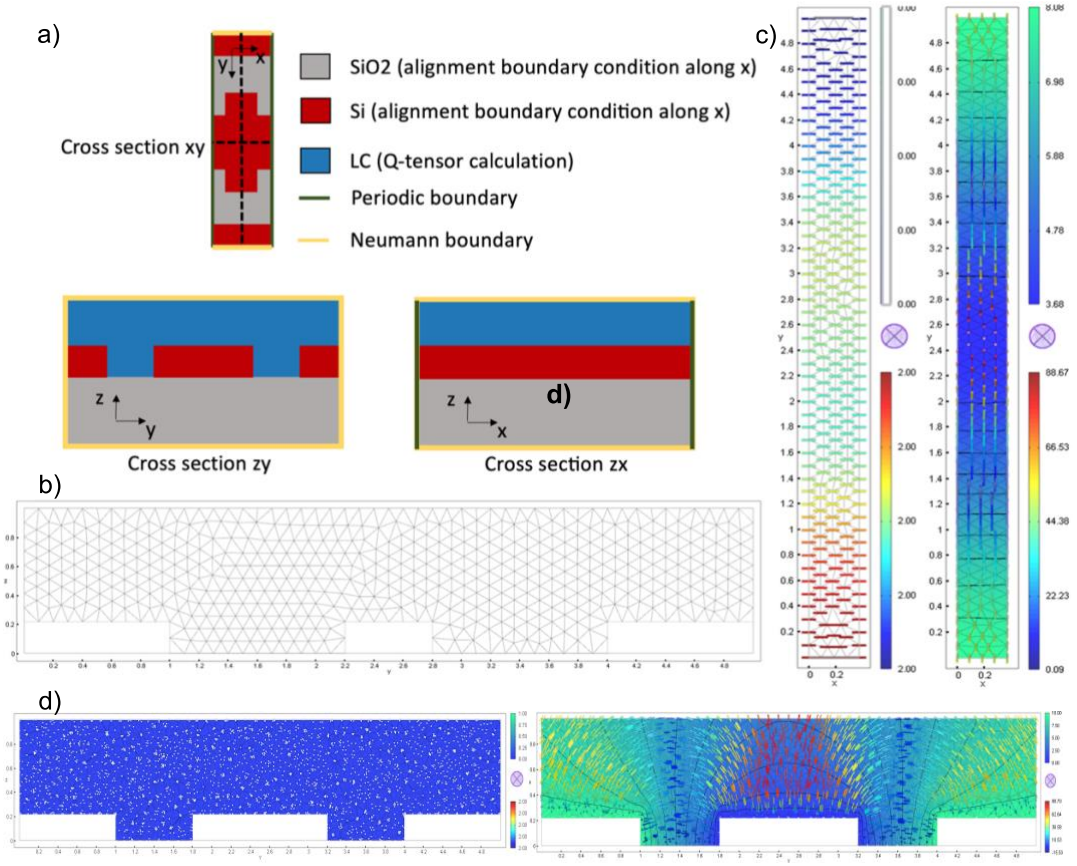

Figure 2: Schematics of LC cladding unit simulated. a) cross sections for one unit cell with boundary conditions. b) Triangular mesh example generated by GID on a slice of LC volume. c) top view for LC

director distribution so that the periodic boundary condition assigned on the left and right sides can be verified. d)left: LC unit when 0V is applied. There are two bar legends on the right side of the figure, where the color of the upper bar legend represents the potential distribution; and the color of the lower bar legend represents the tilt angle of the director. right: 10V is applied.

Finite-Difference Time-Domain (FDTD) Simulations

In this work, we use a commercially available solution (Ansys Lumerical) to solve the 3D Maxwell's equations using FDTD, where a silicon-on insulator bimodal periodic waveguide is simulated, see Figure 3 [4]. The cladding material is designed as a uniaxial diagonal anisotropic permittivity tensor defined by two axes having an ordinary refractive index (n_o=1.5) and other having an extraordinary refractive index (n_e=1.7). We import the director components (n_x, n_y, n_z) obtained from the Q-tensor calculation grid in the software, which can be used to determine how the diagonal permittivity tensor should be rotated at each grid point. The director distribution obtained for the unit cell can be replicated for each period to cover the whole structure.

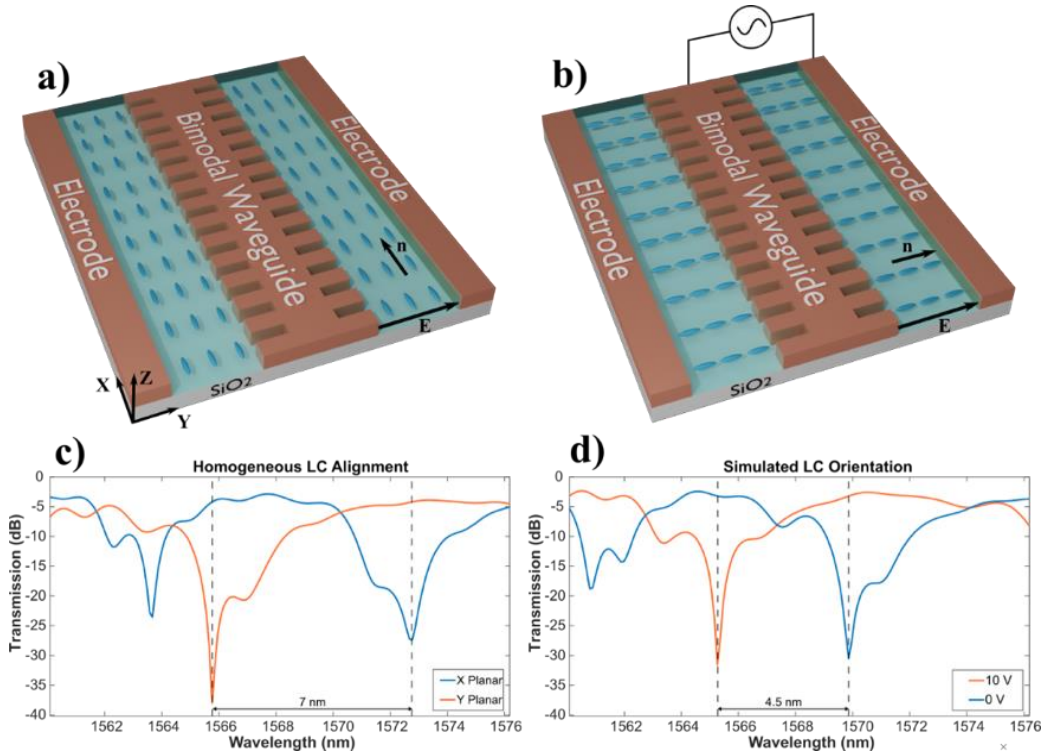

Figure 1: On top, bimodal waveguide operation principle sketch. a) When no voltage is applied the LC director (n) aligns with the longitudinal direction of the waveguide, thus the TE mode will experience $n \approx n_o$. b) LC reorientation due to the applied voltage, provoking that the TE model will experience $n \approx ne$. On the bottom, simulated transmission spectrum for different configurations. c) Homogeneous LC cladding. d) 3D simulated LC orientation.

Optical simulations have been carried out for director distributions corresponding to two voltages: 0 V and 10 V. When no voltage is applied, the director aligns with the longitudinal direction of the waveguide. This means the TE mode will experience the ordinary refractive index of the LC (Figure 1a). When the voltage is increased to 10 V, the LC director aligns with the applied electric field, causing the TE mode to interact with the extraordinary index (Figure 1b). This effect can be seen on the transmission spectra shown in Figure 1d as a shift on the resonance peak position of 4.5 nm. The shift in the

transmission spectra demonstrates that the two propagating modes are not equally affected by the LC director reorientation. This is expected, as the higher order mode has a smaller confinement. We also simulated the transmission spectrum with homogeneous alignment of the same permittivity tensor (Figure 1c) obtaining a significantly greater resonance peak shift (7 nm). These results show that using a uniform alignment as opposed to a 3D director distribution will overestimate the resonance shift.

Conclusions

In this study, we present a methodology to simulate periodic structures in an SOI-platform with a 3D LC cladding. Liquid crystal orientation simulations were done using a Finite Element Method (FEM), where the reorientation of LC under the action of an external electric field is investigated. These spatially varying LC distributions can be imported in a Finite Difference Time Domain (FDTD) solver, enabling us to assess the optical performance impact of the 3D director distribution. A tunable bimodal periodic waveguide is simulated using this procedure showing a resonance peak shift of 5 nm under 10 V.

Acknowledgments

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References

[1] W. Bogaerts *et al.*, 'Programmable photonic circuits', *Nature*, vol. 586, no. 7828, Art. no. 7828, Oct. 2020, doi: 10.1038/s41586-020-2764-0.

[2] L. Torrijos-Morán, A. Brimont, A. Griol, P. Sanchis, and J. García-Rupérez, 'Ultra-Compact Optical Switches Using Slow Light Bimodal Silicon Waveguides', *Journal of Lightwave Technology*, vol. 39, no. 11, pp. 3495–3501, Jun. 2021, doi: 10.1109/JLT.2021.3066479.

[3] L. V. Iseghem *et al.*, 'Low power optical phase shifter using liquid crystal actuation on a silicon photonics platform', *Opt. Mater. Express, OME*, vol. 12, no. 6, pp. 2181–2198, Jun. 2022, doi: 10.1364/OME.457589.

[4] L. Torrijos-Morán, A. Griol, and J. García-Rupérez, 'Slow light bimodal interferometry in one-dimensional photonic crystal waveguides', *Light Sci Appl*, vol. 10, no. 1, Art. no. 1, Jan. 2021, doi: 10.1038/s41377-020-00460-y.

[5] N. J. Mottram and C. J. P. Newton, 'Introduction to Q-tensor theory'. arXiv, Sep. 12, 2014. Accessed: Nov. 13, 2023. [Online]. Available: http://arxiv.org/abs/1409.3542

[6] R. James, E. Willman, F. A. FernandezFernandez, and S. E. Day, 'Finite-element modeling of liquid-crystal hydrodynamics with a variable degree of order', IEEE Transactions on Electron Devices, vol. 53, no. 7, pp. 1575–1582, Jul. 2006, doi: 10.1109/TED.2006.876039.