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ABSTRACT

The paper focuses on the simulation of plasmonic organic hybrid electro/optic modulators. The problem is addressed with two simulation strategies: a *divide et impera* approach based on 2D RF and optical frameworks, and an all-in-one 3D model. The shortcomings and criticalities of both approaches are discussed through a comparison with experimental results from the literature. Possible extensions of the *divide et impera* are envisioned, tracing a viable roadmap towards a computationally sustainable and accurate comprehensive 3D simulation framework.

Keywords: Plasmonics; Mach-Zehnder modulators (MZMs); Plasmonic modulators; Plasmonic-organic-hybrid (POH); Electro-optic effect;

1 INTRODUCTION

Plasmonic organic hybrid (POH) electro-optic (E/O) Mach-Zehnder (MZ) modulators for 1.3 μm and 1.55 μm systems are a topical subject in the framework of silicon photonics integrated platforms [1]. Indeed, they exhibit outstanding modulator performances (albeit with quite large optical insertion losses) thanks to their non-diffraction limited characteristics, nanometer scale cross-sections, micron scale total lengths and exceptional E/O material characteristics [2]. POH modulators exploit polymer-based E/O materials consisting of chromophore molecules dispersed in a host medium, which are previously oriented according to a static poling electric field [3]; modulation of the material refractive index is enabled by imposing an RF electric field to the poled material. This material fills the phase shifters, which are designed to support plasmonic modes. Thanks to the nanometer slot widths, very large RF electric fields can be obtained with low applied voltages, thus enhancing the E/O effect.

It is understood that the simulation of POH E/O modulators requires a multiphysics treatment, where the electro-optic modulation is evaluated from RF electrical simulations and is later used to obtain a complex, position-dependent and anisotropic refractive index profile adopted as input of the optical model. In this view, a simplified model could exploit 2D modal simulations to achieve the modulator static/dynamic response. Yet, such an approach cannot predict some effects, such as undesired power losses related to surface plasmons pertinent to the top/bottom waveguide walls. Describing these details would require a 3D full-wave model of the entire geometry, which is very challenging because of the extremely severe memory and computational requirements. The aim of this work is to present a critical appraisal of the available simulation tools for POH MZ modulators ranging from in-house multiphysics 2D FEM codes [4], [5] to commercial 3D FDTD-based frameworks [6]. The shortcomings of each of these instruments are identified through a comparison with experimental results [7]. The possibility to establish a hierarchy of hybrid 2D-3D models is investigated, with the aim to overcome the limitations of the single approaches.

2 *DIVIDE ET IMPERA* 2D STRATEGY

The *divide et impera* strategy has been applied to the structure sketched in Fig. 1 (left). This shows the 2D cross-section of one of the phase modulators of the MZ interferometer, which consists of a metal-insulator-metal (MIM) waveguide filled with the DLD-164 polymer ($n = 1.83$ at $\lambda = 1.55\,\mu$m [8], total height $h_{\mathrm{DLD}} \simeq 300\,$nm). The gold rails are deposited on a SiO_2 layer, which lies on a Si substrate (not shown in the figure). The slot height h_{slot} is 220 nm, while the width w_{slot} is designed to be quite small, in order to maximize the slot electric field and emphasizing the E/O effect. In particular, the device under study has two different slot widths, namely 100 nm and 90 nm, so that the 0 V operation point does not coincide with the ON state; for properly designed slot widths, these devices are ideal for IQ modulation [1].

The *divide et impera* strategy consists of three fundamental steps. The first is the determination of the poling/modulation electric field, which determines the chromophore orientation. This is obtained from a quasi-static electrical simulation [5], whose output is the position-dependent anisotropic refractive index variation induced by the E/O effect. Then, this becomes the input of a full-wave optical mode simulator [4], which evaluates the RF-voltage-dependent complex refractive index of the plasmonic waveguide. Finally, the static

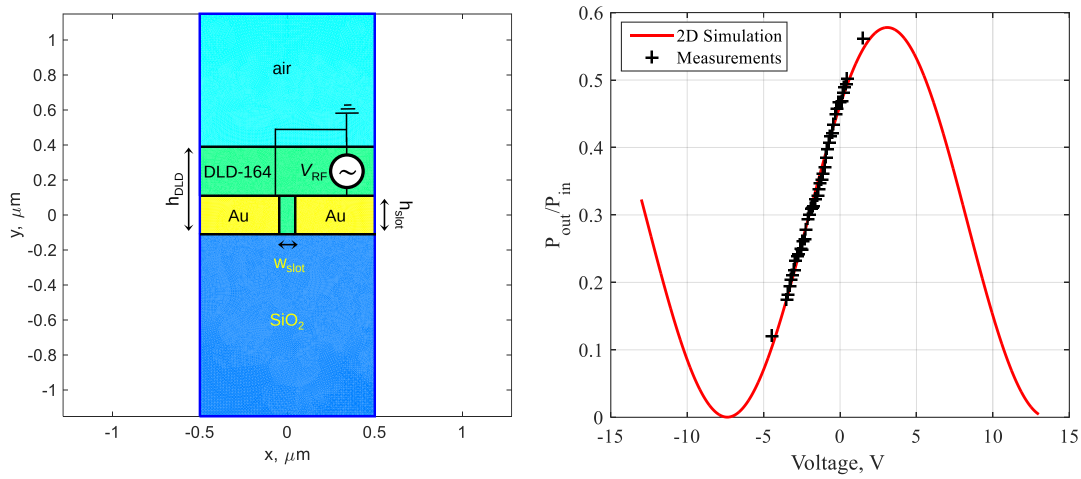

Figure 1. Left: cross-section of the optical simulation, indicating materials and main geometrical dimensions; the $V_{\rm RF}$ voltage generator has been sketched to emphasize the presence of the E/O effect. Right: $P_{\rm out}/Pin$ static response evaluated with the 2D *divide et impera* simulation framework (solid red line) and from an experimental characterization [7].

modulator response is evaluated with simple analytic expressions [9, Sec. 6.4.2]. The results of this approach have been applied to assess the electro-optic coefficient of the device. This has been carried out by using r_{33} to fit the experimental characterization results presented in [7]. Fig. 1 (right) shows the result of the fitting procedure, achieving $V_\pi = 10.5$ V with $r_{33} = 190$ pm/V, which is perfectly compatible with the estimates presented by the ETH group [7].

3 ALL-IN-ONE 3D SIMULATION

Even though the multiphysics *divide et impera* 2D strategy estimates correctly some of the modulator figures of merit, it exhibits several limitations. Indeed, considering the full device sketched in the inset of Fig. 2 (left), the phase modulators are fed by a mode converter, consisting of dielectric-metal tapers, which transforms the input dielectric waveguide (pink) field into plasmonic modes; a dual conversion takes place at the modulator output. Being focused only on the cross-section depicted in Fig. 1 and assuming that all power is coupled into the fundamental plasmonic mode, the 2D approach neglects every aspect of mode conversion, being therefore inadequate to estimate losses due to radiation and/or coupling to surface plasmonic modes, and input/output mismatch. These effects play an important role also in the evaluation of the extinction ratio (ER), which is largely overestimated by 2D models (infinite, for symmetric MZ modulators).

An alternative to the *divide et impera* 2D strategy is the all-in-one simulation of the full MZ POH modulator, whose results are reported in Fig. 2. These plots have been obtained from simulations performed with a commercial 3D finite-difference time-domain (FDTD) solver [6]. A larger V_π, around 14 V, can be noticed at a glance, which is related to the fact that these simulations are optical-only, so that the E/O effect has been included assuming constant static field only in the slot, neglecting fringing/corner effects [2]. The red curve of Fig. 2 (left) reports the power transmission coefficient from the input to the output waveguide, which is a figure of merit comparable to the $P_{\rm out}/P_{\rm in}$ reported in Fig. 1 (right).

The ER has been estimated to be around 6 dB, which is qualitatively compatible with the results shown in Fig. 2 (right), showing the horizontal electric field magnitude in the modulator in OFF (top), half-power (center) and ON (bottom) states. However, this is rather poor compared to the results of the experimental characterization [7]. Still, it is to be remarked that the ER has been measured downstream of mode filters and "long" stretches of optic fiber, which cannot be treated by FDTD for its staggering computational cost. In order to emulate this downstream processing, a correction has been introduced to the power transmission coefficient, multiplying it times the input/output power overlap integral, leading to the blue curve and to the more reasonable 20 dB estimate.

4 CONCLUSIONS AND PERSPECTIVES

This work deals with the simulation of MZ POH modulators. Two simulation approaches are presented, discussing their advantages and limitations. The 2D *divide et impera* strategy is computationally-feasible and provides reasonable estimates of some modulator figures of merit, but it neglects several effects pertinent to mode coupling, which affect the device losses and ER performance. On the other hand, the all-in-one approach is potentially much more realistic, but it comes at the price of extreme computational requirements. Indeed, a standard simulation is performed on a computational box of $4 \times 4 \times 20\,\mu{\rm m}^3$, with uniform mesh cells with 10 nm

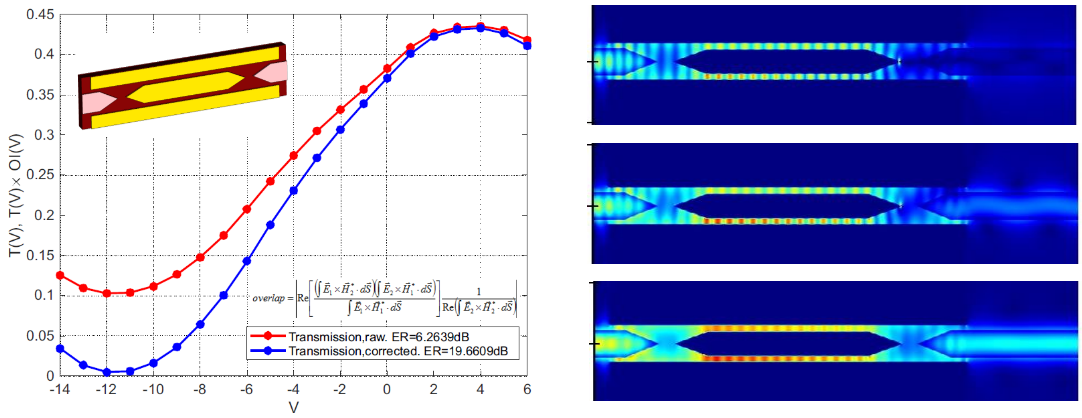

Figure 2. Left: output/input power transmission coefficient simulated with the all-in-one 3D FDTD model; the inset shows the 3D modulator model; the *raw* transmission coefficient (red line) is corrected (blue line) by multiplying it times the output/input power overlap integral (formula in the inset). Right: top view of the middle section of the modulator in the OFF (top), half-power (center) and ON (bottom) states: magnitude of the horizontal field component.

edge, leading to huge memory requirements and long computational times that make it hard even assessing the model convergence with respect to the mesh step and/or the position of the absorbing boundary conditions.

A third approach improving the 2D *divide et impera* at a (relatively) moderate computational payoff could be based on performing a 3D simulation only of the dielectric-plasmonic mode converter, characterizing it with a (in general multimodal) 3-port scattering matrix. In this view, propagation over the plasmonic phase modulators could be evaluated analytically, enabling also the full-wave simulation of traveling modulators.

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