Abstract

In the present zettabyte era, the increasingly growing amount and quality of services provided to a worldwide audience leads to an incessant demand of computational resources for processing and transporting information. Already consolidated in both datacom and telecom contexts, on-chip optical communications are the Holy Grail towards Tbit/s transmission rates with negligible energy consumption. In a framework where scaling and integration are still the most sensitive terms silicon photonics appears as the most natural technological platform to realize low-cost and CMOS-compatible integration of electrical and optical systems.

Specifically, silicon photonics addresses the study and the technological applications of silicon and other group-IV semiconductors as optical medium for generation, transmission, modulation and detection of light.

The cost of production for the integrated circuits makes unfeasible a trial-and-error approach for the development of new devices. In fact, simulation-driven design has become a standard in the industry: it is a low-cost solution capable to provide insights on the inner workings of our device (i.e. carrier densities, electric field distribution). Thanks to such numerical insights new directions and choices can be swiftly explored in the design of the next semiconductor product.

In order to have a quantitative comparison against experimental measurements and/or other theoretical approaches, we require from our model to be an accurate depiction of the physical situation. All this should come at the cost of a reasonable amount of resources (i.e. execution time, RAM).

Drift-diffusion models and Monte Carlo techniques applied to the Boltzmann transport equation (BTE) are the standard approaches in semiconductor modelling. In the drift-diffusion model, the motion of our carriers is described as the sum of two component: a *drift* term describing the electrical current produced by the electrostatic potential $\phi(x)$ and a *diffusion* term proportional to the gradient of concentration of electrons and holes $n(x), p(x)$. Poisson's equation and charge continuity close the drift-diffusion model leading to an effective description of the physics in the semiconductor device based on differential equations. Even more challenging is the solution of multiphysics problems where two or more physical domains interact and must be solved selfconsistently. Consider the case of a photodetector: finite-difference time domain (FDTD) algorithms are employed to solve

Maxwell's equation from the illumination source up to the absorbing region of the detector; the presence of space dependent optical generation profile $G_{opt}(x, y, z)$ will produce a perturbation on the carrier distributions $n(x, y, z)$, $p(x, y, z)$ inducing a variation of refractive index seen by the optical problem. A self-consistent approach is mandatory in this case, unless we can ignore the eventual "feedback" mechanisms on the basis of experimental evidences or theorical proofs simplifying the solution of the multiphysics problem. In such a context, electro-optical simulations of high-speed waveguide-coupled detectors and optical modulators have been performed and presented in this work:

- in the first chapter, we introduce a few concepts on what is silicon photonics and what it can offer in terms of convergence between electrical and optical sub-systems. A brief introduction over two fundamental components of silicon photonics, photodetectors and optical modulators, is given.

- in the second chapter, we describe what a waveguide-coupled photodetector is and how it compares to vertically-illuminated ones. After a short excursus of the technological and technical achievements within scientific literature, results on the coupled optical and electrical simulation are presented. In particular, a more refined description of the Si/Ge heterointerface and a coupled electrooptical simulation of a pin photodetector illuminated using a lateral asymmetric waveguide are presented. On one hand, we discovered the introduction of a thin graded $Si_{1-x}Ge_x$ region to be fundamental to attain good agreement between simulations and experimental results of n-on-p photodetectors; on the other hand, multiphysics simulations confirm the advantage of lateral illumination with respect to butt-coupling solutions when exposed to high-level input optical power.

- in the third chapter, we focus on plasmonic-organic hybrid modulators detailing their advantages over standard implementations. Following a review of the available experimental results and numerical simulations, we present some results on the modelling of plasmonic modulators using commercial electromagnetic solvers. Specifically, simulations of plasmonic slot waveguides loaded with a linear electro-optic polymer and of a plasmonic Mach-Zehnder modulator have been performed. A parametric study of the slot waveguide's dimensions through a finite element method (FEM) modal solver gave us the possibility to leverage semi-analytical models that simplified the design of the Mach-Zehnder modulator. Such design was then validated by means of more complete numerical approaches such as finite difference time-domain (FDTD) or eigenmode expansion (EME).

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