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Simulation in optoelectronics : state of the art and trends

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Abstract

Due to increasing needs of high performance devices for optical communication, CAD tools and especially numerical simulation have become a key point of the design. In this paper, we examine the latest methods used in these fields, and try to project their evolution during the next years.

Introduction

Development and huge progress in optical telecommunications during the last 20 years have led to a high diversity of electro−optical functions realized through various structures and geometries. This goes from emission devices (laser diodes) to amplification (integrated optical amplifiers, Er doped fibers, ...), filtering (coupler, Bragg reflectors, MachZehnder, ...) and reception components (PIN photodiode, APD, etc...). Moreover, in order to increase the performances, these functions are now being integrated into *Photonic Integrated Circuits* (PIC) which increases the complexity of the design and requires then highly versatile CAD tools, able to to handle a large set of physical effects and coupling phenomena between optical, electrical and thermal behaviors.

A. Specificities of CAD in optics

One of the main difficulties of CAD−tools in optics lies in the fact that, unlike the case of electronic design, there is no powerful analysis tool as the "equivalent electric schematic". Some laboratories have developed identical methods (based on microwave CAD−tools in most cases) [1] but the main drawbacks of these methods lie in phenomena such as light scattering, radiated loss and unwanted interactions between different parts of the same integrated device which are poorly taken into account.

This lack of a "schematic" general−purpose CAD tool leads to use the numerical solving of Maxwell equations (or their derivatives) as the main CAD−tool for a very large class of devices. Here arise problems due to the geometric dimensions : Integrated Optical (IO) devices are often several millimeters long, several tenths of microns wide and several microns high, while the wavelength is around one micron : this means a volume of the device at least a million time the size of the typical variation cell ! Solving the Maxwell equations under such conditions needs then to make assumptions that will reduce the complexity of the problem but also the validity area of the method. The world of numerical simulation in optics is therefore divided in a great number of specialized algorithms, each one bringing an answer for a class of devices and it often happens that the same device has to be examined through different methods in order to obtain a full overview of its performances.

One can separate optoelectronic devices in many classes. First we will distinguish passive devices, where the behavior of the guided light depends only on the geometry and the material characteristics, from active devices, where more complex optical functions are achieved through coupled interactions between optical field and electrostatic field or free carriers.

Passive devices

This class of devices has been thoroughly investigated and a lot of numerical methods are now in competition for use as CAD tools. Most of these methods are based on the well−known *Beam Propagation Method* (BPM) which consists in rewriting the Helmholtz equation which rules the propagation of the electric (or magnetic) field. This equation, given by :

$$rot\,(rot\,\vec{E}) = \omega^2 n^2\,\vec{E} \qquad (1)$$

can be reformulated as a propagation equation, assuming that the field is mainly propagating forward in the z−direction :

$$\frac{\partial}{\partial z}\,\vec{E} = \mathbf{A}\;\vec{E} \qquad (2)$$

where **A** is the propagation operator. Differences between *Fast Fourier Transform−BPM* (FFT−BPM), *Finite Differences BPM* (FD−BPM), *Finite Elements−BPM* (FE−BPM) lie in the choice of the mathematical vectorial space used to discretize the field which leads to differences in computation and accuracy. Examples of these techniques can be found in [2],[3].

Another extension of this method, also called ME−BPM for *Mode Expansion−BPM*, is based on the decomposition of the wave on the local 2D propagation modes of the structure and is much more suited for devices containing large z−invariant parts than classical BPMs, but can become very inefficient for devices containing continuous varying parts. The propagation operator is calculated through by multiplying transfer matrix between modes of contiguous sections. Many examples have shown the efficiency of this method [4].

Nevertheless, in order to get reasonable computation time for a real CAD tool and even in spite of the increasing computation power of workstations, the computation time of a 3D vectorial propagation in an optical device is around some hours on a workstation. The problem has then to be reduced from tri−dimensional (3D) to two−dimensional (2D), most often using the *Effective Index Method* which assumes that the behavior of the field in one transverse direction (in general the vertical direction) is well−known and does not vary significantly along the propagation. The limitations induced by this assumption (problems in taking into account the vectorial effects, poor accuracy for vertical tapers) and recent state of the art works show clearly that future CAD−tools in this field will be full 3D and vectorial [5],[6].

The other key point of this kind of simulation lies in the knowledge of the refractive indices of materials, which is in general good for binary materials but can become very poor for quaternary alloys such GaInAsP, widely used in IO. This point is critical when the behavior of a device such as a filter or a Bragg reflector depends on a variation of 10^{-4} of the refractive index [7].

to sum up, we can say that, even if a lot a work has still to be done mainly for 3D vectorial propagation, a lot of efficient and reliable algorithms are now available in CAD for passive optical devices and have shown a real predictive power for designing and optimizing structures.

Active devices

Much more complicated is the situation in active devices, e.g. devices mixing optical and electrical phenomena in order to achieve high−level optical functions such as emitting, switching, filtering and so on. What is more, like electronic components, nowadays actice devices have to be investigarted on time and frequency scales arround and over 1 GHz which adds also the time discretization problem for dynmaical simulations. Among active devices, one can first make the distinction between devices involving carrier transport or not.

B. Electro−optic coupling

Devices which do not involve free carriers transport, for example electro−optic couplers, require most of the time the resolution of a 2D guided mode equation coupled to a Poisson equation (3); in this case, the coupling results from the dependency of the refractive index with the electrostatic field :

$$\begin{aligned} rot\,(rot\,\vec{E}) &= \omega^2 n^2_{refr}\,\vec{E} \\ div(\epsilon\,\vec{\nabla}\phi\,) &= q\,(n - p - N_D^+ + N_A^-) \qquad (3) \end{aligned}$$

This type of simulation can be easily handled by a two−dimensional finite elements solver [8] and the influence of the electrostatic field on the refractive index can be modelled by a linear (Pockels effect) or non−linear effect (Kerr effect). Computation time of such simulation is form some minutesto an hour (for dynamical simulation) on a classical workstation.

This model used to simulate the behavior of the device is relatively simple compared to devices including electronic transport, but the accuracy of the results will depend strongly on the precise knowledge of the coefficients involved in both effects. Like in the case of the refractive indices, the main problem of this simulation lies in then in obtain reliable values of these coefficients, for a large set of materials, from direct measurements or from comparisons with simulation.

C. Lasers and optical amplifiers

On the contrary, in active devices involving carrier transport as semiconductor lasers or semiconductor optical amplifiers (SOA), the complexity and the variety of the phenomena increase drastically. Such devices include 3D electronic transport, heat diffusion, optical propagation which are coupled through radiative and stimulated recombinations, variation with the temperature of all the electronic band parameters and photonic rate equation for lasers.

Moreover, in most cases these phenomena would require a full 3D approach as for example in the case of the B.R.S.

laser (Buried Rib Structure) where the direction of the light propagation is perpendicular to the current lines of the electronic transport (fig. 1). However, due to memory requirements and computation time constraints, the problem must be in general transformed in a two-dimensional coupled problem.

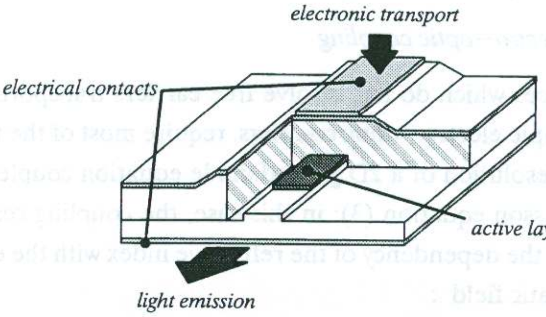

fig. 1 : structure of the BRS semiconductor laser

In one of these approaches, the model used for simulating such a device is constituted by a 2D drift-diffusion system coupled to a 2D mode computation in a vertical plane (transverse to the propagation axis) [9]: Poisson equation and classical drift-diffusion equations for free carrier transport (4,5) are coupled to an Helmholtz equation which replaces a 3D light propagation. The third direction is represented through a photon-rate equation (6) :

$$
\begin{aligned}
&div(\epsilon \vec{\nabla}\phi) = q\,(n - p - N_D^+ + N_A^-) \\
&-q\frac{\partial n}{\partial t} + div\,\vec{J}_n = qU \qquad (4) \\
&q\frac{\partial p}{\partial t} + div\,\vec{J}_p = -qU \qquad (5) \\
&rot\,(rot\,\vec{\boldsymbol{E}}) = -\,n_{refr}^2\,\frac{\partial^2\vec{\boldsymbol{E}}}{\partial t^2} \\
&G(n)\,S_{phot} - \frac{S_{phot}}{\tau_{ph}} + \beta\,U_{rad} = 0 \qquad (6)
\end{aligned}
$$

Such a model can also be improved by taking into account the heat generation and diffusion (7), which alter significantly the behavior of the laser [10] :

$$C\frac{\partial T}{\partial t} + div(-\kappa\vec{\nabla}T) = \vec{\nabla}E\,.\,\vec{\nabla}J \qquad (7)$$

In spite of the reduction of dimensionality from 3D to 2D, the computation time for the I-V characteristic of a standard structure is around a few hours on a workstation and around one hour on a fast supercomputer. This mean that we cannot consider this kind of software as a CAD-tool and that its use is still restrained to the verification of some global assumptions for lower precision models.

Another approach consists in simulating the propagation coupled to the electronic transport in a vertical plane including the propagation axis [11]. In this case, the propagation simulation must take into account the backward propagated wave which excludes explicite propagation techniques as FFT- or FD-BPM.

D. Quantum-well structures

Development of new epitaxial growths techniques has opened the way to the design of structures including multi-quantum wells, improving the performances in terms of polarization sensitivity, laser threshold, carrier mobilities. To be accurately taken into account, carrier localization in such structures requires the use of the Schrödinger equation (8) :

$$\frac{\hbar^2}{2m}\Delta\Phi_n + V(\vec{r})\,\Phi_n = E_n\,\Phi_n \qquad (8)$$

In this case the carrier density is no longer represented only by a Boltzmann or a Fermi-Dirac distribution but two distinct populations of electrons (resp. holes) must be considered : the first is the classical "bulk" population being transported by a drift-diffusion-type current and the second is the population located in the wells, whose evolution is governed by the exchanges with the "bulk" population and the holes. The expression of the optical gain in the active layer is also changed to take into account the detailed optical transitions between energy levels of carriers.

One can find in the literature simulations including this type of transport carried out for semiconductor optical amplifiers [11] or semiconductor lasers [12].

The recent use of new materials like non-InP-lattice matched GaInAsP, in order to lower the threshold current, requires to compute the effects of a the strain on the device performances. In these structures, the strain causes indeed the valence band to split between light and heavy hole bands and an accurate simulation of the optical transitions needs to solve a coupled system including the Poisson equation and a Schrödinger equation with an Luttinger-Kohn Hamiltonian [13].

This type of model shows perfectly the limitation of nowadays simulations : in order to obtain reliable results, it needs a lot of constants (strain parameters, Hamiltonian coefficients, capture and emission times) for new materials (non-lattice matched) and which are very difficult to get directly from measurements. In the same time, each simulation takes a considerable computation time, even on the fastest workstation. Efficiency in this field can then only be achieved through the inter−mixing of different algorithms : 1D simulation including the more detailed physical effects (Schrödinger, strains, ...) and creating tabulated data for 2D simulation which could take into account the coupling with the propagation mode of the light and even 3D software for simulating the variation of the the light intensity and carrier density along the cavity (spatial hole burning).

Several years ago, the use of heterostructures with different III−V materials in electronic devices, in order to improve their performances, has opened the way to a real "band gap engineering" which created a lot of constraints on simulation tools and required the use of new algorithms and numerical techniques. We can see almost this happening today with the introduction of strained multi−quantum wells in a large number of optical devices : the main challenge in this field will be for the next years to develop algorithms and also material database for simulating this new "strain engineering".

conclusion

Models and simulation techniques used in opto−electronics have strongly improved during the last decade and now cover a wide range of devices and phenomena. But the designer willing to use a versatile and efficient CAD tool is still facing two main problems :

First the number of simulation algorithms has incredibly increased (FFT−BPM, FD−BPM, Finite Differences, Finite Elements, Mixed Finite Elements, Method of Lines, etc...) and each of these algorithms is best suited for a device or a class of devices. We can almost say that all the "basic blocks" (optical propagation, electronic transport, Schrödinger equation. ...) of a complete simulation tool exist but still need to be assembled for each class of device. A future target CAD software is likely not to be constituted around one or two algorithms but rather will have at its disposal a whole library (a tool box) with standard inputs−outputs allowing the user to "build" his simulation software for each device. Moreover a special effort has to be done for a comprehensive treatment of the electro−optical behavior of strained multi−quantum wells.

The second problem is related to the great variety of materials used in opto−electronics. New technological approaches like the "band−gap engineering" and now the "strain engineering" moved the emphasis from the "classical" III−V binary alloys such as GaAs or InP to ternary or quaternary alloys, whose characteristics are not well known. Furthermore, improvement of growth epitaxial techniques allows the designers to use non−lattice matched materials (for example in multi−quantum wells) in order to reduce or erase the polarization sensitivity of the devices. An enormous work of measurements, classification, comparisons, has then to be done in this field in order to end up with a reliable efficient and predictive CAD tool in optoelectronics.

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