

Nonlinear Algorithms for the Quantum Mechanical Simulation of Electroabsorption

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An overview of nonlinear simulations of electroabsorption modulators and their physical and numerical requirements is given. The algorithm includes all important aspects, like excitonic and carrier-dependent effects, a self-consistent treatment and quantum mechanical behaviour.

Keywords: Electroabsorption modulator, excitons, density matrix, absorption, quantum-confined Stark effect

Introduction

Although electroabsorption modulators (EAM) become increasingly important, there is a huge gap between requirements and state of the art semiconductor technology and simulation. The high complexity of the nonlinear behaviour of modulators is still a challenge, which is not sufficiently accepted.

The presented algorithm is one of the most extensive tools to model EAMs and to analyze nonlinear behaviour. It includes the most important optoelectronic effects, which are essential for the modulator's performance, e.g. the quantum-confined Stark effect and the Franz-Keldysh effect, and also accounts for carrier-dependent effects. Therefore coupled descriptions of electrical and optical properties are needed. A drift-diffusion model and quantum corrections primarily characterize the electrical parameters, while a density matrix formalism, instead of \vec{k} -space solutions, determines the optical behaviour. Density matrices allow boundary conditions in real space and provide efficient calculations.

This procedure includes the excitonic effect, all important quantum mechanical effects, nonlinear carrier-dependent effects and enables self-consistent and time-dependent methods.

Solution in \vec{k} -space

If the bound states of the calculated structure are known, it is possible to gain a first estimation of the absorption [1]. The exciton equation in k -space is solved by expanding the exciton states in terms of subband states, which result from band structure calculations in the envelope function approximation (EFA) [2, 3] by solving the stationary Schrödinger equation using a kp -Hamiltonian. Discretisation generates an eigenvalue problem, which can be efficiently solved. Unfortunately, the calculation of the matrix elements makes this procedure time consuming. The exciton wave function, on the other hand, is used for solving the density matrix equation, which determines the complex dielectric function. This directly results in the refractive index and chirp parameter [1].

For an accurate description of the optical properties of EAMs Wannier-excitons must be included. Therefore, the following Schrödinger equation is solved to determine the exciton states Ψ_{ex}

$$\mathbf{H}_{ex}(z)\Psi_{ex} = E_{ex}\Psi_{ex}, \quad (1)$$

where $\mathbf{H}_{ex}(z)$ is the effective Hamiltonian including a Coulomb term. To Ψ_{ex} an expansion is applied, which is based on the eigenfunctions resulting from the single-particle Schrödinger equation. The numerical evaluation of this expansion is very time-consuming.

The density matrix for interband processes is used to calculate the optical properties. It determines the complex dielectric function and renders a tedious Kramers-Kronig transformation to calculate the refractive index change unnecessary. We expand the coherent electron-hole

wavefunction in terms of the exciton wavefunction. The emerging integrals in \vec{k} -space lead to tedious band structure calculations, which makes this method unsuitable for nonlinear computations. Therefore, an alternative algorithm is applied.

Density matrix in real space

The solution of the density matrix in real space yields a more accurate description of excitonic effects and provides the following advantages.

The Coulomb singularity can be resolved analytically by polynomial finite elements [4]. Bound, quasi-bound and free states are as well modelled as all electric field dependent effects like quantum confined Stark effect (QCSE), Franz-Keldysh effect (FKE) and Wannier-Stark effect (WSE) and mixtures of these. The density matrix formalism allows to calculate both real and imaginary part of the susceptibility. The finite coherence length can be used to terminate the calculation space efficiently by open boundary conditions like the perfectly matched layers (PML) [5].

The stationary equation for the coherent electron-hole amplitude Y

$$(\mathbf{H}_{eh} - \hbar\omega - j\hbar\Gamma_{eh})Y = \mu\vec{E}, \quad (2)$$

with the Hamiltonian \mathbf{H}_{eh} for parabolic bands, which is used for general quantum well structures and superlattices allowing spatially dependent effective masses for electrons and holes

$$\begin{aligned} \mathbf{H}_{eh} = & -\frac{\partial}{\partial z_e} \frac{\hbar^2}{2m_e} \frac{\partial}{\partial z_e} - \frac{\partial}{\partial z_h} \frac{\hbar^2}{2m_h} \frac{\partial}{\partial z_h} - \frac{\hbar^2}{2m_r} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \right) \\ & + E_c(z_e) - E_v(z_h) - \frac{e^2}{4\pi\epsilon\sqrt{r^2 + (z_e - z_h)^2}}, \end{aligned} \quad (3)$$

the driving electric field \vec{E} , the optical dipole matrix element μ and a phenomenologic dephasing rate Γ to describe the reduction of Y by scattering processes, is solved by applying a nodal finite elements (FE) approach. m_e and m_h are the position dependent electron and hole effective masses in z direction, $m_r = 1/(m_{e||}^{-1} + m_{h||}^{-1})$ is the reduced mass in radial direction. The electron and hole band energies are labelled E_c and E_v , respectively.

The main advantage of this approach is that the Coulomb singularity is modelled exactly for polynomial base functions [4]. Due to this the approach presented is more accurate.

The optical polarization \vec{P} and the optical susceptibility χ result from an integration over relative coordinates r and z

$$\vec{P}(Z) = \iint \mu Y(Z, z, r) r dr dz, \quad \chi = \frac{P}{\epsilon_0 E}. \quad (4)$$

In typical waveguide modulators the induced optical field only slightly differs, thus a first order perturbation theory is appropriate to calculate a complex effective dielectric function

$$\epsilon_{\text{eff}} = \frac{\int (1 + \chi(Z)) E^2(Z) dz}{\int E^2(Z) dz} \quad (5)$$

from the material susceptibility χ .

Semiconductor Equations

The single particle equations for electron-electron and hole-hole interactions are approximated by a semi-classical drift-diffusion model (DDM). Therefore, a system containing Poisson's

equation (6), the continuity equations (7) and (8) and carrier transport equations of the drift-diffusion model with an additional quantum correction (9) and (10) is solved in a decoupled manner to determine the electrical properties of the structure:

$$\nabla \cdot (\epsilon \nabla \Psi) = -e(p - n + N_D - N_A), \quad (6)$$

$$\nabla \cdot \vec{J}_e - e \frac{\partial n}{\partial t} = eR, \quad n = N_e F_{1/2}(\eta_e), \quad (7)$$

$$\nabla \cdot \vec{J}_h + e \frac{\partial p}{\partial t} = -eR, \quad p = N_h F_{1/2}(-\eta_h), \quad (8)$$

$$\vec{J}_e = -en \mu_e \nabla \Phi_e, \quad (9)$$

$$\vec{J}_h = -ep \mu_h \nabla \Phi_h. \quad (10)$$

These equations contain the self-consistent potential Ψ , the carrier concentrations n (electrons) and p (holes) and the concentrations of completely ionized acceptors N_A and donors N_D . Further, the difference between recombination and generation rates R , the carrier current densities \vec{J}_e and \vec{J}_h for electrons (e) and holes (h), respectively, and the mobilities μ_e and μ_h are as well used as the quasi Fermi potentials Φ_e and Φ_h . N is the effective density of states, $F_{1/2}$ the Fermi integral of order 1/2 and carrier densities are calculated for Fermi distributions. To account for quantum mechanical effects the classical potential is corrected by the Bohm potential, which smoothes the carrier densities. The Poisson equation (6) is solved by the Gummel algorithm [6, 7].

Coupling of electronical and optical properties and nonlinear effects

To investigate nonlinear behaviour and saturation effects the optical properties have to be coupled to the semiconductor equations to account for carrier dependent phenomena. This can be realized by an additional generation rate, which is determined by the exciton equation. The saturation terms in the source terms of the density matrix equation, neglected in Eq. (2), lead to an optical generation of carriers. This generation can be accounted for in the continuity equations (7) and (8) - a coupling of the electrical and the optical system can be realized this way. Consequently, an additive generation-recombination rate R_{opt} can be derived

$$R_{opt} = -E^2 \text{Im}(\chi) \frac{\epsilon_0}{\hbar} \quad (11)$$

leading to a nonlinear calculation [8].

Saturation effects can be modelled due to the coupling of electrical and optical system by including R_{opt} . A small band gap and a small density of states cause a fully occupied band near the band edge, the so-called Burstein-Moss effect, which appears in terms of a modified Coulomb term. As a counterpart to the Burstein-Moss effect, a reduction of the band gap has to be regarded. Concerning high carrier concentrations, this follows from exchange terms in the interband density matrix equations.

For an accurate analysis of delay times and saturation phenomena transient models are implemented as explicit algorithms, Crank-Nicolson schemes and fully implicit algorithms.

Calculation

A laser-modulator structure (InGaAlAs/InP) is shown, where both regions contain the same active regions (Fig. 1). Fig. 2 shows the absorption spectra (averaged over the respective active region) for modulator mode and the contributions of the laser and modulator to it. The laser region has a huge damping impact on the light in modulator mode, as absorption in this region is very effective.

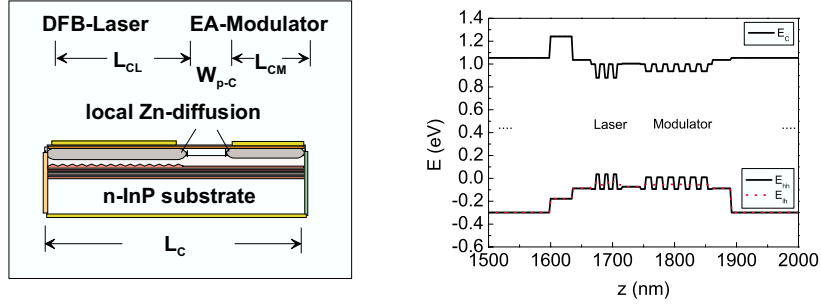


Fig. 1. Left: MESA-Structure of the Laser-Modulator Device; Right: Band Structure of the Active Region.

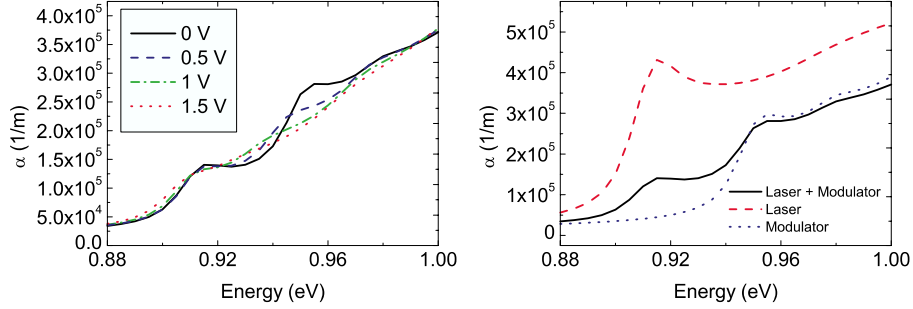


Fig. 2. Left: Absorption Spectra of the Device for Modulator Mode; Right: Contributions of Laser and Modulator to the Absorption

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