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Modeling of quantum dot lasers with microscopic treatment of Coulomb effects

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ABSTRACT. We present a spatially resolved semiclassical model for the simulation of semiconductor quantum-dot lasers including a multi-species description for the carriers along the optical active region. The model links microscopic determined quantities like scattering rates and dephasing times, that essentially depend via Coulomb interaction on the carrier densities, with macroscopic transport equations and equations for the optical field.

1. INTRODUCTION

Due to many advantages, such as low threshold currents and improved robustness of operation, semiconductor quantum dot (QD) lasers have become increasingly interesting for telecom applications. The need for a detailed understanding of the physics involved and for optimization of such devices makes them subject for theoretical investigations, comprising modeling and numerical simulation. A suitable model used for the simulation of such devices constitutes a complex multiscale problem and has to cover many important physical effects.

On the coarsest scale, classical carrier transport through the bulk part of the device can be described by a macroscopic model, which are the drift-diffusion equations in our case. Additionally, a semiclassical description of the optical field by Maxwell equations is required. Usually, by selfconsistently coupling of both the electronic and the optical model via the optical gain on one hand, and via the rate of spontaneous and stimulated recombination on the other hand, a self-consistent picture for the spatial distributions of the carriers and the field intensity (Bandelow et al, 2003) is achieved.

However, due to the quantum confinement of carriers on the scale of a few nanometers in QD active regions, c.f. Fig. 1, processes like optical gain, scattering and recombination of carriers have to be described by a microscopic model. The carrier-carrier scattering via Coulomb interaction, that dominates at high carrier densities (Nielsen et al, 2004; Nilsson et al, 2005; Lorke et al, 2006) and which we will exclusively take into account within this paper, causes nonradiative, Auger-like transitions between QDs and carrier reservoirs such as bulk and wetting layer (WL) states. Thereby, the dynamics of the laser can be strongly influenced by density dependent scattering rates (Viktorov et al, 2006). Also the optical transitions between the QD electron and hole states, that result in the optical gain, will be modified by the Coulomb interaction. This is reflected by a density dependend dephasing time (Lorke et al, 2006; Dachner et al, 2010), which modifies the optical gain. The active region of our considered device comprises optically active QDs grown on a 2D WL as shown in Fig 1a. We will restrict to two-level QDs possessing only a single electron and only a single hole state, see Fig. 1c.

The paper is organized as follows: We present in Section 2 a spatially resolved multi-species electronic model for QD lasers. In Section 3 we address the microscopic calculation of the Coulomb-assisted carrier-carrier scattering and the dephasing processes occurring in the model. We demonstrate this approach by calculations of scattering rates and dephasing times for a two-level QD system, including the calculation of the optical gain.

2. MULTI SPECIES MODEL

In our model we differ between bulk carriers, reservoir carriers, here taken to be confined in a two-dimensional WL, and carriers that are localized in the quantum dots as schematically shown in Figs. 1a and 1c. The bulk carriers are freely roaming through the

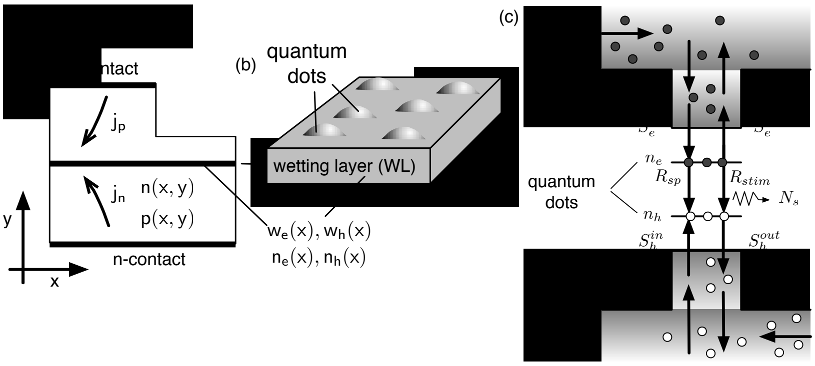

FIGURE 1. (a) Scheme of transverse cross-section of an edge-emitting QD laser with a QD-WL active region that contains lens-shaped QDs (b). (c) Scheme of scattering and recombination processes in the quantum dot active region described by the multi-species model. Carriers are injected from the bulk into the wetting layers and enter the quantum dots by Coulomb scattering. There they contribute to the stimulated recombination.

layers in devices as depicted in Fig. 1c and are described by classical drift-diffusion equations. The two-dimensional transport of the carriers confined in the WL is described by in-plane drift-diffusion equations, whereas the occupation of the QD-states is governed by rate equations for localized states. All these equations are coupled to each other by corresponding carrier-exchange rates and by the electrostatic potential via the Poisson equation. The injection of the bulk carriers into the wetting layers, as depicted in Fig. 1, is described by phenomenological capture-escape models (Grupen and Hess, 1998; Steiger et al, 2008). For the capture-escape process from the wetting layer into the quantum dots we use scattering rates derived from a microscopic model for the dominating Auger-like processes at high carrier densities, which have their physical origin in Coulomb-scattering. The conceptual approach to describe the carriers in low-dimensional nanostructures by a partition of the carrier density into different species has been proposed by Steiger et al (2008) for the simulation quantum-well and quantum-wire based optoelectronic nanostructures.

For edge-emitters we can restrict our considerations to a transverse cross section $\Omega \subset \mathbb{R}^2$ of the device, as schematically shown in Fig.1a. In order to simplify the presentation of our model we consider in the following the case of QD-lasers containing only a single QD optical active layer. We denote the Nabla operator with respect to $\mathbf{r}_t = (x,y) \in \Omega$ by ∇, and its in-plane part with respect to the in-plane coordinate $\mathbf{r}_\parallel = (x,0)$ along the QD layer by $\nabla_\parallel$. The bulk carrier densities of the electrons and holes are denoted by n and p and are defined on the whole cross-section Ω of the device, see Fig. 1a. The carrier densities of the electrons and holes confined in the WL and in the QDs are denoted by w_e, w_h and n_e, n_h, respectively. The WL densities w_e and w_h and QD occupation densities n_e and n_h are sheet densities depending only on the in-plane coordinate $\mathbf{r}_\parallel$, see Fig. 1a. The evolution of the carrier densities is governed by the following system of equations:

$$(1) \qquad -\nabla\cdot(\varepsilon_0\varepsilon_s\nabla\varphi) = q(C - n^{tot} + p^{tot}),$$

$$(2) \qquad \frac{\partial n}{\partial t} - \frac{1}{q}\nabla\cdot\mathbf{j}_n = -R - C_n^{3,cap},$$

$$(3) \qquad \frac{\partial p}{\partial t} + \frac{1}{q}\nabla\cdot\mathbf{j}_p = -R - C_p^{3,cap},$$

$$(4) \qquad \frac{\partial w_e}{\partial t} - \frac{1}{q}\nabla_\parallel\cdot\mathbf{j}_{we} = -\tilde{R}^{nr} + C_n^{2,cap} - \left[S_e^{in}(N^{QD} - n_e) - S_e^{out} n_e\right]\frac{N^{tot}}{N^{QD}} - R_{sp}^{WL},$$

$$(5) \qquad \frac{\partial w_h}{\partial t} + \frac{1}{q}\nabla_\parallel\cdot\mathbf{j}_{wh} = -\tilde{R}^{nr} + C_p^{2,cap} - \left[S_h^{in}(N^{QD} - n_h) - S_h^{out} n_h\right]\frac{N^{tot}}{N^{QD}} - R_{sp}^{WL},$$

$$(6) \qquad \frac{\partial n_e}{\partial t} = S_e^{in}(N^{QD} - n_e) - S_e^{out} n_e - R_{\mathrm{stim}} - R_{\mathrm{sp}},$$

$$(7) \qquad \frac{\partial n_h}{\partial t} = S_h^{in}(N^{QD} - n_h) - S_h^{out} n_h - R_{\mathrm{stim}} - R_{\mathrm{sp}}.$$

The net charge density, given by the sum over the the local distributions of the respective electron and hole species, together with the doping profile C, enters the Poisson equation (1) for the electrostatic potential φ, where q is the elementrary charge and ε_s is the static permittivity. The bulk electron and hole current densities $\mathbf{j}_n$ and $\mathbf{j}_p$, as well as those for the WL, $\mathbf{j}_{we}$ and $\mathbf{j}_{wh}$, are defined in the usual way by gradients of corresponding quasi Fermi-potentials, i.e. $\mathbf{j}_n = -q\mu_n n\nabla\varphi_n$ and $\mathbf{j}_{we} = -q\mu_{we} w_e \nabla_\parallel \varphi_{we}$, c.f. (Steiger et al, 2008). $C^{3,cap}$ describes the injection from the bulk into the WL by phenomenological capture-escape rates according to Grupen and Hess (1998). $C^{2,cap}$ are the corresponding charge-conserving counterparts in the WL equations. $S_{e/h}^{in}$ and $S_{e/h}^{out}$ are scattering rates describing the capture and escape processes from the WL into the QDs. These scattering rates depend nonlinearly on w_e and w_h, see Section 3 and Fig. 2a. N^{tot} is twice the total density of QDs grown on the WL and N^{QD} is twice the sheet density of resonant QDs. The rates of spontaneous recombination in the WL and QDs are denoted by R_{sp}^{WL} and R_{sp}, respectively. The rate of stimulated recombination in the QDs is denoted by R_{stim} and defined by

$$(8) \qquad R_{\mathrm{stim}} = \frac{v_g}{L} g(\omega)|\Xi_0|^2 N_s,$$

where L is the length of the laser, v_g is the group velocity and $\Xi_0(\mathbf{r}_t)$ refers to the normalized transverse main mode profile. In the case of stable transverse waveguiding and longitudinal single-mode operation we work with the balance equation

$$(9) \qquad \dot{N}_s = v_g(2\Im m\beta - \alpha_0)N_s + r^{sp}.$$

for the numbers of photons N_s, where $\Im m[\beta]$ is the modal gain given by the imaginary part of the corresponding eigenvalue β of the transverse waveguiding problem, α_0 are all longitudinal losses by scattering into other modes (radiation modes, e.g.) including outcoupling losses. The spontaneous emission rate into the mode is denoted by r^{sp}. For further details we refer to (Bandelow et al, 2003).

The material gain caused by the interband polarization from the QDs has the form:

$$(10) \qquad g(\omega) = -\frac{\omega}{n(\omega)c}\frac{|d_{vc}|^2}{L_0}(N^{QD} - n_h - n_e)\int \frac{\Gamma_2(\varepsilon, w_e, w_h)}{(\varepsilon - \hbar\omega)^2 + \Gamma_2(\varepsilon, w_e, w_h)^2}\, G(\varepsilon)\, d\varepsilon,$$

where $\Gamma_2 = \hbar/T_2$ (11) is the homogeneous broadening of the gain defined by the dephasing time T_2, and $G(\varepsilon)$ is the (Gaussian-shaped) distribution of the QD transition energy, which causes inhomogeneous broadening. In Eq. (10) $n(\omega)$ is the refractive index, c is the speed of light, d_{vc} the dipole matrix element of the QD transition, L_0 is a normalization length.

If one neglects bulk/WL carrier transport and assumes spatially homogenous WL and QD densities, Eq.s (1)–(9) reduce to a set of rate equations. Such type of rate-equation models have been applied for the analysis of the electron and hole dynamics of edge-emitting QD lasers (Malic et al, 2006; Lüdge et al, 2008; Lüdge and Schöll, 2009).

3. Coulomb scattering between quantum dot and wetting layer states

The calculation of the scattering rates S^{in} and S^{out} as found in Eqs. (4)-(7), as well as of the dephasing time entering Eq. (10) of the resonant QD transition, has been treated by density matrix theory in the limit of the second order Born approximation. The description results in a nonlinear dependence of these scattering rates and of the dephasing time on the WL carrier density (Nielsen et al, 2004; Nilsson et al, 2005; Lorke et al, 2006; Malic et al, 2007). For precise calculations several scattering channels between the QD and WL have to be included, as in particular pure dephasing processes for the calculation of T_2 (Lorke et al, 2006). The dephasing time determines the homogeneous line width of the single QD gain, additionally broadened by an inhomogeneous distribution of QDs, see Eq. (10).

To describe $S^{in/out}$ we use a Hamiltonian according to Nielsen et al (2004) containing free carrier energies of both quantum dot and wetting layer states and carrier-carrier interaction via the Coulomb matrix element $V_{abcd} = \int d^3r \int d^3r' \phi_a^*(\mathbf{r})\phi_b^*(\mathbf{r})V(\mathbf{r}-\mathbf{r}')\phi_c(\mathbf{r}')\phi_d(\mathbf{r})$. The latter is calculated with QD and WL-OPW-wavefunctions as in Nielsen et al (2004), where a, b, c and d are compound indices denoting all possible QD and WL states. This includes the highest WL valence subband, the lowest WL conduction subband and both the QD valence and conduction ground states, all doubly degenerate due to spin. In the following we will use the indices i and j to denote states restricted to the QDs.

To derive the scattering contribution, we consider the temporal evolution of density matrices ρ_{ab}, since they determine all dynamical quantities in Eqs. (4)-(7). For consistency with our semiclassical description of the WL used in the multi-species model we assume quasi-equilibrium for the WL states by using Fermi-distributions in the following. The parameters used for the numerical calculations of scattering rates and dephasing times are near to Lorke (2008) for shallow QDs. Additionally, we used the approximation that the width of the WL equals to the height of the QDs and to L_0 in Eq. (10), which applicable to the considered lens-shaped QDs embedded in the WL.

The diagonal elements $\rho_a := \rho_{aa}$ of the density matrix are the occupation probabilities of the states a. Our EOM for the occupation probabilities of QD states has the same form as in Malic et al (2006). The determination of S^{in} and of S^{out} are next to Nielsen et al (2004), but we included screening in the static limit of the Lindhard-formula (Haug and Koch, 2004). The resulting scattering rates are depicted in Fig. 2a (for room temperature) and show a nonlinear dependence on the WL carrier density. The dephasing time $T_2 = \hbar/\Gamma_2$ of the QD polarization ρ_{ij}, $i \neq j$, has in the markovian limit the form

$$
\begin{aligned}
\Gamma_2 =\pi \sum_{a,b,c} \Big\{ & W_{abic}\Big(W_{icab} - W_{icba}\Big)\left[\rho_c(1-\rho_b)(1-\rho_a) + (1-\rho_c)\rho_b\rho_a\right]\delta(\varepsilon_a+\varepsilon_b-\varepsilon_c-\varepsilon_i) \\
& + W_{jabc}(W_{bcja} - W_{cbja})\left[\rho_b\rho_c(1-\rho_a) + (1-\rho_b)(1-\rho_c)\rho_a\right]\delta(\varepsilon_j+\varepsilon_a-\varepsilon_b-\varepsilon_c) \\
& - 2\Big(W_{aiic}W_{jcaj} - W_{aiic}W_{jcja} - W_{iaic}W_{jcaj}\Big)\ \left[(1-\rho_c)\rho_a\right]\delta(\varepsilon_a-\varepsilon_c) \\
& - \Big(W_{abij}W_{jiba}\Big)\ \left[\rho_j(1-\rho_b)(1-\rho_a) + (1-\rho_j)\rho_b\rho_a\right]\delta(\varepsilon_a+\varepsilon_b-\varepsilon_j-\varepsilon_i) \\
& - \Big(W_{jibc}W_{cbij}\Big)\ \left[\rho_b\rho_c(1-\rho_i) + (1-\rho_b)(1-\rho_c)\rho_i\right]\delta(\varepsilon_j+\varepsilon_i-\varepsilon_b-\varepsilon_c)\Big\}.
\end{aligned}
\tag{11}
$$

Here W_{abcd} denotes the screened Coulomb matrix elements. In previous publications (Kim et al, 2010; Dachner et al, 2010) an approximation of this expression by contributions possessing a similar formal structure as the in- and out-scattering terms (first two lines) has been used, which leads to smaller dephasing times. For the numerical evaluation of Γ_2 in this paper all contributions in (11) have been considered. Results for the calcuation of the dephasing time are depicted in Fig. 2b. The gain spectra for our example QD-WL

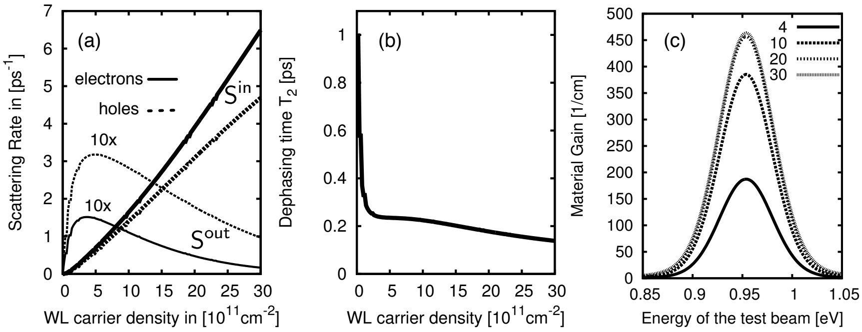

FIGURE 2. Calculated (a) Coulomb scattering rates for electrons (solid) and holes (dotted), (b) dephasing time T_2, in dependence on the WL carrier density. (c) gain spectra for WL densities $4, 10, 20, 30 \cdot 10^{11}\mathrm{cm}^{-2}$. For the calculation of the scattering rates Auger-like processes according to Malic et al (2007) have been considered, together with an inhomogenoues broadening FWHM of 60 meV. $w_e = w_h$ always assumed.

structure are depicted in Fig. 2c. As a result of the Coulomb interaction, they exhibit a saturation behaviour with increasing carrier density.

4. CONCLUSION

A semiclassical, spatially resolved, multi-species model for the simulation of semiconductor QD lasers has been presented. The electronic model comprises the carriers in the bulk, in the wetting layer, and in the QDs, governed by suited transport equations. The coupling between the equations for the wetting layer densities and the equations for the QD densities are determined in particular by microscopically calculated scattering rates between these species. This electronic model is selfconsistently coupled to equations for the optical field, where in addition a microscopically determined dephasing time enters via the optical gain. In effect these microscopically calculated quantities become dependent on the carrier densities in a nonlinear way. This nonlinear behavior is expected to influence the dynamic properties of such devices, as e.g. their modulation response (Lüdge et al, 2008). The presented model goes beyond the existing approaches with respect to the following two aspects: First, in pure rate-equation models the influence of a spatial inhomogenous current injection, of the electrostatic interaction via the Poisson equation, and of the spatial inhomogenous stimulated recombination is neglected. Second, compared to other existing models with spatial resolution, we cover the impact of important QD-WL Coulomb interaction on the scattering rates and on the optical gain by microscopic calculations.

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