Light-Matter Interaction in NEGF Simulations of Intersubband-Emitting Devices

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***Abstract*—The light-matter interaction for the case of stimulated intersubband emission was included through appropriate selfenergy into nonequilibrium Green's function formalism to simulate electrical and optical characteristics of quantum cascade laser above the lasing threshold.**

***Index Terms*—nonequilibrium Green's function method, electron-photon selfenergy, light-matter interaction, quantum cascade laser, intersubband transitions**

I. Introduction

For optoelectronic devices, the light-matter interaction is essential. In nonequilibrium Green's function (NEGF) formalism [1], it can be included either through appropriate selfenergy [2–4] or time-dependent (ac) potential incorporated into device Hamiltonian [5]. For unipolar devices, utilizing intersubband transitions, only the "ac" approach was used [5–7]. This approach requires solving the full set of NEGF equations for several higher harmonic of fundamental frequency what generates huge numerical load. On the contrary, the selfenergy approach generates only little additional load as the light-matter selfenergy (like other selfenergies) is included into NEGF equations for the steady state. In this paper, the selfenergy approach is used to perform simulations of quantum cascade laser (QCL).

II. Model

In QCLs, light is emitted due to intersubband transitions occurring in the conduction band. Therefore, one-band effective mass Hamiltonian, parametrized for the in-plane momentum k, provides the sufficient description [8]:

$$H = \frac{-\hbar^2}{2}\frac{d}{dz}\frac{1}{m(E,z)}\frac{d}{dz} + V(z) + \frac{\hbar^2 k^2}{m(E,z)}, \tag{1}$$

where z is the coordinate along the transport direction and other symbols have the usual meaning. In (1), mixing with valence bands is taken into account by the use of energy (E) dependent effective mass m. The potential $V(z)$ includes both the variation of the conduction band edge and the Hartree term of the electron-electron interaction. For such a formulation, the Green's functions have 4 arguments, i.e., $G(z, z', E, k)$. The calculations are made in the position basis: the base vectors are defined by the points discretizing the Hamiltonian (1). As QCL core is periodic, the structure subjected to calculations is limited to a bit more than one QCL period connected to the leads that reliable imitate device periodicity [8, 9]. The formulations for scattering self-energies were taken from [1] for LO-phonon, interface roughness, ionized impurity, and alloy disorder scatterings, whereas for the acoustic phonons we use the energy-averaged approximation described in [8].

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In QCLs, the radiative intersubband transitions are stimulated by the z-polarized light propagating along the y-axis. The electromagnetic field can be described in terms of the vector potential $\mathbf{A} = [0\ 0\ A_z]$ which can be related to photon flux Φ through the Poynting vector $S = \Phi E_\gamma = 2nc\epsilon_0 E_\gamma^2 \hbar^{-2}|A_z|^2$, where n is material refractive index. To the first order in A_z, the perturbation theory gives the interaction Hamiltonian [2]:

$$H_1 = \frac{e\mathrm{i}}{\hbar} A_z[H, z], \tag{2}$$

which can be used in the derivation of selfenergies $\Sigma^{<,\mathrm{R}}$: for monochromatic field with the photon energy $E_\gamma = h\nu$

$$\begin{aligned}\Sigma^{<,\mathrm{R}}(z, z', E, k) = \iint dz dz' H_1(z)[G^{<,\mathrm{R}}(z, z', E{+}E_\gamma, k) \\ + G^{<,\mathrm{R}}(z, z', E - E_\gamma, k) H_1(z')].\end{aligned} \tag{3}$$

The above formulation differs from that in [2] in that the terms responsible for spontaneous emission are omitted. The selfenergies were included into the steady state NEGF formalism like other selfenergies: the Dyson and Keldysh equations were iterated until the selfconsistent solution was achieved. Then, the gain/absorption was calculated from the linear response to a small ac field perturbation, like in [10].

III. Results

The model described in Sec. II was tested on GaAs/AlGaAs QCL described in [12]. The self-consistent band structure of one device period, laser levels, and the corresponding wavefunctions are shown in Fig. 1. The full NEGF-based analysis of the electronic transport in this device, however without electron-photon interaction, has already been presented in [11]. The results that include this interaction are presented in Figs. 2 and 3. In Fig. 2, the calculated gain-flux and current-flux dependencies are compared with the relations predicted by the 2-state rate equations model [6, 7]:

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$$g(\Phi) = \frac{g(0)}{1 + eg_0 d\Phi}, \quad J(\Phi) = J(0) + edg(\Phi)\Phi, \qquad (4)$$

where g is the gain at energy E_γ, J is the current density, g_0 is the gain coefficient, and d is the period length. In case of the gain, the agreement with semi-classical result is excellent when the value g_0 is taken from the calculations in the off state (see Fig. 3). For the current density, the agreement is poorer, but still very good: note that no fitting parameters were used when drawing the lines. The agreement found in Fig. 2 proves that the calculations of the optical gain (ac field perturbation) are consistent with the calculations of electronic transport (scattering electron-photon selfenergies).

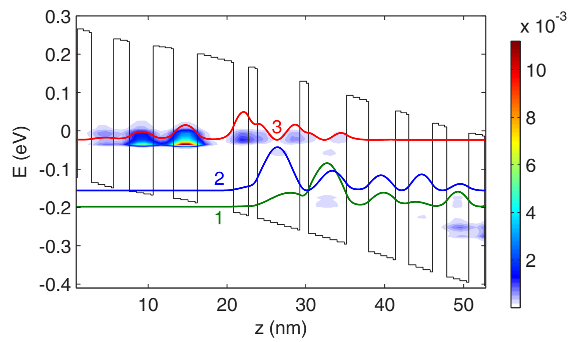

Figure 1. Conduction band profile, laser (3, 2) and depopulating (1) levels wavefunctions (modulus squared) and electron density in units $\mathrm{eV}^{-1}\mathrm{nm}^{-3}$ (contour color plot) calculated with the NEGF method.

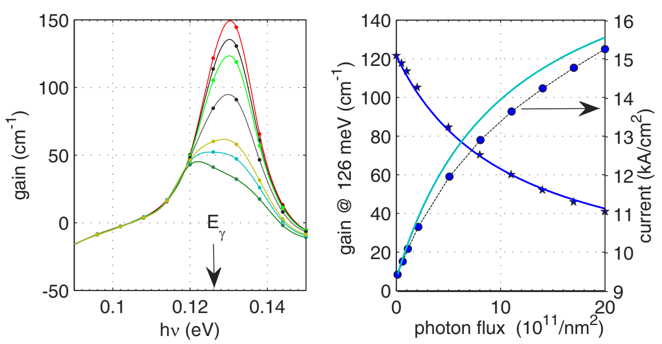

Figure 2. (left) Gain spectra for the increasing photon flux (up-to-down) set at $h\nu = E_\gamma = 126$ meV. (right) Gain at $h\nu = E_\gamma$ and current density as a function of photon flux set at $h\nu = E_\gamma = 126$ meV calculated with the NEGF method (symbols). Lines in the right plot are drawn according to (4).

The calculations have been done for the number of bias voltages with electron-photon interaction turn off or on. For the latter case, the monochromatic field with energy $E_\gamma = 0.126$ eV was used, and flux Φ was increased until the gain was clamped to its threshold value $g_{\mathrm{th}} \cong 60\ \mathrm{cm}^{-1}$ described by the total losses [12]. Then, the light power leaving the cavity through one of the mirrors was related to Φ as [6, 7]:

$$P = (1 - R)N_p d\Phi E_\gamma, \qquad (5)$$

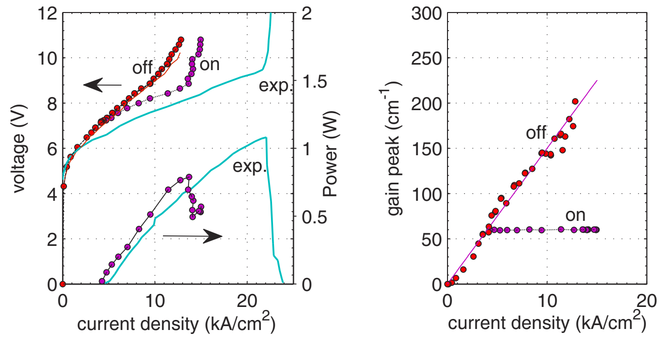

Figure 3. (left) Current-voltage and light-current characteristics calculated with or without electron-photon selfenergies included into NEGF formalism; (right) gain peak for these two cases. The slope of the line approximating the data in the off state is $g_0 = 12.9$ cm/kA. Lines show experimental data [12].

where $R = 0.27$ is the facet reflectivity and N_p is the number of periods in a cascade. Results are shown in Fig. 3 and compared with the experimental data of [12]. The agreement is not bad, especially if we take into account that the only adjustable parameter of the model is the roughness of the interfaces which was assumed as $\frac{1}{3}$ of the monolayer spacing. The observed differences are probably due to the overestimated losses assumed in the model as well as the doping of the core in the real samples that might have been higher than the nominal value $4 \times 10^{17}\mathrm{cm}^{-3}$ assumed in the simulations.

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