Calculation of quantum well laser gain spectra

W.W.Chow

Sandia National Laboratories, Albuquerque, NM 85718-0601

wwchow@somnet.sandia.gov

A.Girndt and S.W.Koch,

Department of Physics and Material Sciences Center,
Philipps University, Renthof 5, 35032 Marburg, Germany

Abstract: This paper describes a method for calculating gain spectra of quantum well laser structures. The approach is based on the Semiconductor Bloch equations, with Coulomb correlation effects treated at the level of quantum kinetic theory in the Markovian limit. Results obtained from applying this method to an InGaN quantum well laser are presented.

OCIS codes: (160.6000) Semiconductors, including MQW; (140.5960) Semiconductor lasers; (140.3430) Laser theory

References

1. B. Zee, "Broadening mechanism in semiconductor (GaAs) lasers: limitations to single mode power emission," *IEEE J. Quantum Electron.* **QE-14**, 727 (1978).
2. M. Yamada and Y. Suematsu, "Analysis of gain suppression in undoped injection lasers," *J. Appl. Phys.* **52**, 2653 (1981).
3. W. W. Chow, P. M. Smowton, P. Blood, A. Girndt, F. Jahnke and S. W. Koch, "Comparison of experimental and theoretical GaInP quantum well gain spectra," *Appl. Phys. Lett.* **71**, 157 (1997).
4. M. Lindberg and S. W. Koch, "Effective Bloch equations for semiconductors," *Phys. Rev.* **B38**, 3342 (1988).
5. H. Haug and S. W. Koch, *Quantum Theory of the Optical and Electronic Properties of Semiconductors*, 3rd ed. (World Scientific, Singapore, 1994).
6. W. W. Chow, S. W. Koch and M. Sargent III, *Semiconductor-Laser Physics* (Springer Verlag, Berlin, 1994).
7. T. Rappen, U-G Peter, M. Wegener and W. Schäfer, "Polarization dependence of dephasing processes: A probe for many-body effects," *Phys. Rev.* **B49**, 10774 (1994).
8. F. Rossi, S. Hass and T. Kuhn, "Ultrafast relaxation of photoexcited carriers: The role of coherence in the generation process," *Phys. Rev. Lett.* **72**, 152 (1994).
9. A. Knorr, S. Hughes, S. W. Koch, R. Indik, M. Mlejnek, R. Binder, J. V. Moloney, "The influence of electron-hole Scattering on linear gain spectra," *Solid.State Commun.* **100**, 555 (1996).
10. W. W. Chow, A. Knorr, S. Hughes, A. Girndt and S. W. Koch, "Carrier correlation effects in a quantum-well semiconductor laser medium," *IEEE J. Sel. Top. Quantum Electron.* **3**, 136 (1997).
11. H. Amano, M. Kito, K. Hiramatsu and I. Akasaki, "P-type conduction in Mg-doped GaN treated with low-energy electron beam irradiation (LEEBI)," *Jpn. J. Appl. Phys.* **28**, L2112 (1989).
12. S. Nakamura, M. Senoh, S. Nagahama, N. Iwasa, T. Yamada, T. Matsushita, Y. Sugimota and H, Kiyoku, "Room-termperature continuous-wave operation of InGaN multi-quantum-well structure laser diodes," *Appl. Phys. Letts.* **69**, 4056 (1996).

13. S. L. Chuang and C. S. Chang, "$\vec{k}\cdot\vec{p}$ method for strained wurzite semiconductors," *Phys. Rev.* **B54**, 2491 (1996).

14. A. F. Wright and J. S. Nelson, "Consistent structural properties for AlN, GaN and InN," *Phys. Rev.* **B51**, 7866 (1995) and references.

15. S. J. Jenkins, G. P. Srivastava and J. C. Inkson, "Simple approach to self-energy corrections in semiconductors and insulators," *Phys. Rev.* **B48**, 4388 (1993).

16. S. H. Wei and A. Zunger, "Valence-band splittings and band offsetsof AlN, GaN and InN," *Appl. Phys. Letts.* **69**, 2719 (1996).

17. F. Jain and W. Huang, "Modeling of optical gain in In/gaN-AlGaN and $\mathrm{In}_x\mathrm{Ga}_{1-x}\mathrm{N}$ quantum-well lasers," *IEEE J. Quantum Electron.* **32**, 859, (1996).

To design quantum well lasers for an expanding range of applications, it is necessary to be able to predict their gain spectra accurately. Gain calculations often assume the effective decay rate approximation, [1, 2] where polarization dephasing effects due to carrier collisions are described by a lineshape function. The dephasing rate, which determines the width of the lineshape function, is an input to the calculation. This widely used approach has been successful in explaining several experimental behaviors of laser devices. However, the phenomenological treatment of carrier collision effects cannot reproduce certain important features of the experimental gain spectrum that are important in advanced semiconductor lasers, such as vertical-cavity surface emitting lasers, wide band gap lasers, and monolithic master-oscillator power-amplifier devices. Specifically, the effective decay rate approximation leads to inaccuracies in the predictions of the gain or absorption in the neighborhood of the transparency carrier density, the general shape of the quantum well gain spectrum, and the spectral shape changes with changing carrier density. [3] Equally important is the limitation to the predictive capability because of the need to treat the dephasing rate as an input parameter.

This paper describes a more detailed treatment of collision effects in a semiconductor gain medium, that involves extending the Hartree-Fock treatment of many-body Coulomb effects to include contributions from the next higher order correlations. By following a procedure similar to that resulting in the Semiconductor Bloch Equations [4, 5, 6] we obtain the equation of motion for the microscopic polarization, [7, 8, 9, 10]

$$\begin{aligned}\frac{d}{dt}p_{\vec{k}}^{\nu_e,\nu_h} &= -i\omega_{\vec{k}}^{\nu_e,\nu_h}p_{\vec{k}}^{\nu_e,\nu_h} - i\Omega_{\vec{k}}^{\nu_e,\nu_h}\left(n_{\vec{k}}^{\nu_e}+n_{\vec{k}}^{\nu_h}-1\right)\\ &\quad -\left(\Gamma_{\vec{k}}^{\nu_e}+\Gamma_{\vec{k}}^{\nu_h}\right)p_{\vec{k}}^{\nu_e,\nu_h}+\sum_{\vec{q}}\left(\Gamma_{\vec{k},\vec{q}}^{\nu_e}+\Gamma_{\vec{k},\vec{q}}^{\nu_h}\right)p_{\vec{k}+\vec{q}}^{\nu_e,\nu_h}\quad . \end{aligned} \tag{1}$$

Present in (1) is the Hartree-Fock contribution leading to the renormalization of the transition frequency

$$\omega_{\vec{k}}^{\nu_e,\nu_h}(N)=\hbar^{-1}\left[\varepsilon_{e,\vec{k}}^{\nu_e}+\varepsilon_{h,\vec{k}}^{\nu_h}+E_{g,0}+\Delta\varepsilon_X^{\nu_e,\nu_h}(N)\right]\ , \tag{2}$$

where

$$\Delta\varepsilon_X^{\nu_e,\nu_h}=\sum_{\vec{q}}\left(V_q^{\nu_e,\nu_e,\nu_e,\nu_e}n_{\vec{k}}^{\nu_e}+V_q^{\nu_h,\nu_h,\nu_h,\nu_h}n_{\vec{k}}^{\nu_h}\right)\ , \tag{3}$$

is the exchange contribution to the renormalized band gap energy. The Hartree-Fock contributions also result in a renormalized Rabi frequency

$$\Omega_{\vec{k}}^{\nu_e,\nu_h}(N)=\frac{1}{\hbar}\left(\mu_{\vec{k}}^{\nu_e,\nu_h}E+\sum_{\vec{q}}V_q^{\nu_e,\nu_h,\nu_h,\nu_e}p_{\vec{k}+\vec{q}}^{\nu_e,\nu_h}(N)\right)\ , \tag{4}$$

where $\mu_{\vec{k}}^{\nu_e,\nu_h}$ is the dipole moment and E is the laser electric field. Equations (3) and (4), contain the Fourier transform of the bare (unscreened) Coulomb potential energy (MKS)

$$V_q^{\nu,\nu',\nu'',\nu'''} = f_q^{\nu,\nu',\nu'',\nu'''} \frac{e^2}{2\varepsilon_b A q} \ , \tag{5}$$

where e is the electron charge, ε_b is the background permittivity, and A is the area of the quantum well layer. The form factor

$$f_q^{\nu,\nu',\nu'',\nu'''} = \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dz' u_\nu(z) u_{\nu'}(z') e^{-q|z-z'|} u_{\nu''}(z') u_{\nu'''}(z) \tag{6}$$

accounts for the effects of the finite quantum well thickness and potential, where $u_n(z)$ is the quantum well eigenfunction. Carrier-carrier correlations give rise to the last two terms in (1), which describe polarization dephasing and screening. There is a diagonal contribution with

$$\begin{aligned}\Gamma_{\vec{k}}^{\nu} &= \sum_{\nu'} \sum_{\vec{q},\vec{k}'} \frac{2\pi}{\hbar} \left(W_q^{\nu,\nu',\nu',\nu}\right)^2 D\left(\varepsilon_{\vec{k}}^{\nu} + \varepsilon_{\vec{k}'}^{\nu'} - \varepsilon_{\vec{k}+\vec{q}}^{\nu} - \varepsilon_{\vec{k}'-\vec{q}}^{\nu'}\right) \\ &\quad \times \left[n_{\vec{k}+\vec{q}}^{\nu}\left(1 - n_{\vec{k}'}^{\nu'}\right) n_{\vec{k}'-\vec{q}}^{\nu'} + \left(1 - n_{\vec{k}+\vec{q}}^{\nu}\right) n_{\vec{k}'}^{\nu'} \left(1 - n_{\vec{k}'-\vec{q}}^{\nu'}\right)\right] \ , \end{aligned} \tag{7}$$

where $D(\Delta) = \delta(\Delta) + i\pi^{-1}\mathcal{P}(\Delta)$, and $\mathcal{P}$ denotes the principal value. There is also a nondiagonal contribution that couples polarizations of different $\vec{k}$'s, with

$$\begin{aligned}\Gamma_{\vec{k},\vec{q}}^{\nu} &= \sum_{\nu'} \sum_{\vec{k}'} \frac{2\pi}{\hbar} \left(W_q^{\nu,\nu',\nu',\nu}\right)^2 D\left(\varepsilon_{\vec{k}+\vec{q}}^{\nu} + \varepsilon_{\vec{k}'-\vec{q}}^{\nu'} - \varepsilon_{\vec{k}}^{\nu} - \varepsilon_{\vec{k}'}^{\nu'}\right) \\ &\quad \times \left[\left(1 - n_{\vec{k}}^{\nu}\right)\left(1 - n_{\vec{k}'}^{\nu'}\right) n_{\vec{k}'-\vec{q}}^{\nu'} + n_{\vec{k}}^{\nu} n_{\vec{k}'}^{\nu'} \left(1 - n_{\vec{k}'-\vec{q}}^{\nu'}\right)\right] \ . \end{aligned} \tag{8}$$

The screened Coulomb potential in (7) and (8) is $W_q^{\nu,\nu',\nu',\nu} = V_q^{\nu,\nu',\nu',\nu} \varepsilon_b/\varepsilon_q$, where ε_q is the dielectric function calculated using the static Lindhard formula. [5] We limit our discussion to the small signal gain, where the carrier populations, $n_{\vec{k}}^{\nu}$ are assumed to be Fermi-Dirac distributions that are inputs to the calculations. Also, we neglect the exchange contributions to (7) and (8), as well as carrier-phonon scattering effects.

The polarization equations are solved numerically for the steady state solution at an input laser field and carrier density. Using semiclassical laser theory, the intensity gain G is given by [6]

$$G = -\frac{2\omega}{\varepsilon_0 n c V \mathcal{E}} \,\mathrm{Im}\left(\sum_{\nu_e,\nu_h,\vec{k}} \left(\mu_{\vec{k}}^{\nu_e,\nu_h}\right)^* p_{\vec{k}}^{\nu_e,\nu_h} e^{i\omega t}\right) \ , \tag{9}$$

where $\mathcal{E}$ is the slowly varying electric field amplitude, ω is the laser frequency, ε_0 and c are the permittivity and speed of light in vacuum, n is the background refractive index, and V is the active region volume.

To illustrate the above approach, we choose the example of an InGaN quantum well laser. Lasers and light emitting diodes that are based on group-III nitride compounds are interesting because they can potentially operate in the visible and ultraviolet wavelength regions.[11, 12] Group-III nitride compounds are characterized by

#2664 - $15.00 US
Received September 15, 1997; Revised February 11, 1998

wide band gaps, as well as high exciton binding energies. Because of the latter, we suspect that Coulomb effects are considerably more important in these compounds that in conventional near-infrared III-V laser compounds. Figure 1 shows the computed spectra for a 2nm $In_{0.2}Ga_{0.8}N/GaN$ quantum well structure and different carrier densities. We use a 6×6 Luttinger-Kohn Hamiltonian and the envelope approximation[13] to compute the hole energy dispersions and optical dipole matrix elements. Input parameters are the bulk wurtzite material parameters.[14, 15, 16] Only the TE gain is shown because the TM gain is negligible in the wurtzite structure for the carrier densities considered.

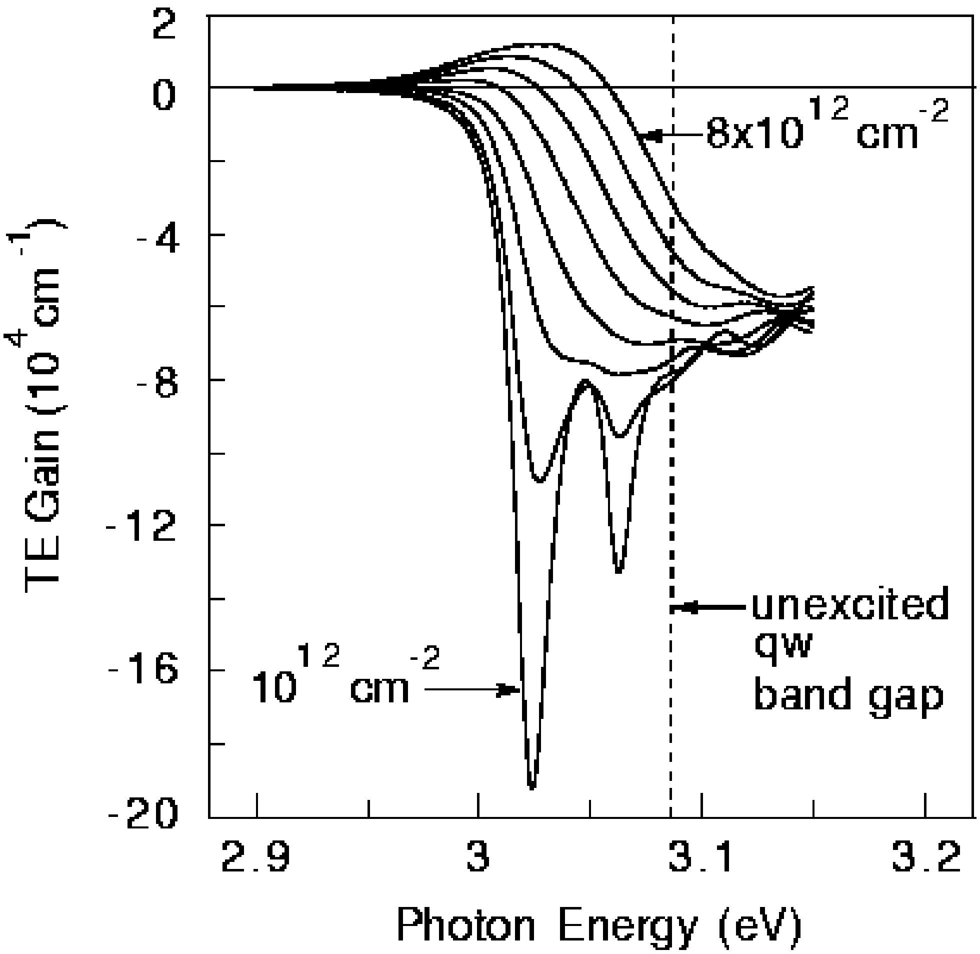

Figure 1. Calculated TE gain spectra for a 2nm wurtzite $In_{0.2}Ga_{0.8}N/GaN$ quantum well at T = 300K and densities N = 10^{12} to 8×10^{12}cm^{-2}, in increments of 10^{12}cm^{-2}.

The spectra describe the transition from low electron and hole densities, where excitons are important, to high carrier densities, where an interacting electron-hole plasma determines the gain medium properties. Note that the excitonic effects are present not because of an *ad hoc* inclusion of excitonic transitions into a free-carrier theory, as is the case in phenomenological models.[17] Rather, they are due to the Coulomb interactions included systematically in the Hamiltonian for the electron-hole system. The presence of exciton resonance at the high temperature and carrier density of $T = 300K$ and $N \simeq 2 \times 10^{12} cm^{-2}$, as well as the large red shift in the gain peak with respect to the unexcited quantum well band edge are evidence of strong Coulomb effects. Figure 2 shows the gain portion of the spectra in more detail. The theory predicts a gradual bulk-like rise in gain with increasing photon energy, and the blue shift in the gain peak with increasing excitation. These features are due to contributions from the nondiagonal Coulomb correlations, and therefore, are not predicted in effective decay rate models.

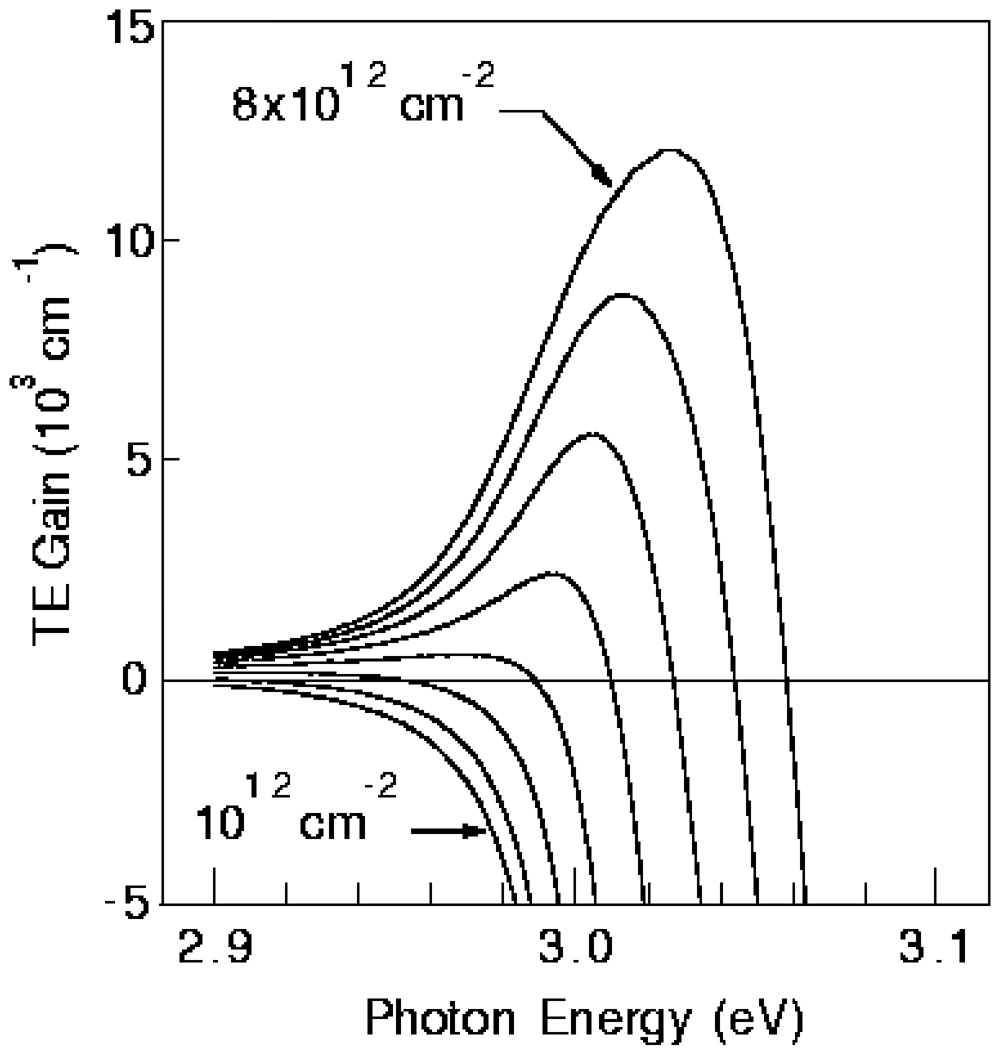

Figure 2. Expanded view of the gain portion of the spectra shown in Fig. 1.

In summary, this paper describes a method for computing quantum well gain spectra, that is based on the Semiconductor Bloch Equations, with carrier collision effects treated at the level of quantum kinetic theory in the Markovian limit. The present approach improves on previous calculations by providing (a) a non-perturbative treatment of Coulomb enhancement effects and (b) a consistent description of collision effects. The latter results in the successful explanation of important features of the experimental gain spectrum, [3] that was not possible with the effective decay rate approximation. The former leads to a more accurate treatment of plasma and excitonic effects, which is important for the description of a new and important class of semiconductor lasers, i.e., those involving group-III nitride compounds.

This work was supported in parts by the U. S. Department of Energy under contract No. DE-AC04-94AL85000, the Deutsche Forschungsgemeinschaft (Germany), the Leibniz Prize and AFOSR-F49620-97-1-0002.

Received September 15, 1997; Revised February 11, 1998