Calculation of gain-current characteristics in ZnCdSe-ZnSe quantum well structures including many body effects

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The gain-spontaneous recombination characteristics have been calculated for a 40 Å $Zn_{0.8}Cd_{0.2}Se$-ZnSe quantum well including many body effects. We examine the effect of the inclusion of the Coulomb enhancement on the gain spectra and the gain-current relationship. We show that, in the absence of the Coulomb enhancement, the threshold current density of a 340 μm 40 Å $Zn_{0.8}Cd_{0.2}Se$-ZnSe quantum well laser is underestimated by approximately 40% and the lasing wavelength overestimated by 4 nm. Our calculation of the scattering lifetime for the first electron-heavy hole transition gives a lifetime varying between 29 and 37 fs, and shows that the carrier-phonon scattering mechanism in II-VI quantum wells is more dominant than in III-V materials. We also comment on the effect the neglect of Coulomb enhancement has on the calculation of leakage currents in a laser at threshold.

Recent advances in II-VI technology have led to the realisation of room temperature, cw blue-green laser diodes.[1–3] Problems with ohmic contacts, material quality and doping are actively being researched. Computer modelling of device structures is a useful tool in these studies. The effects of doping[4] and leakage current[5] have already been studied in this way. The foundation of such calculations is the determination of the material gain in the laser's active region as a function of the quasi Fermi levels or the carrier populations. Initial calculations of gain in II-VI quantum well structures used the free carrier approximation,[5–8] but the effect of the electron and hole Coulomb interaction has been shown to have a significant effect in the calculation of bulk II-VI material gain.[9] Commercial laser diodes are likely to use quantum wells due to their increased performance over bulk active region lasers. In this paper we illustrate the importance of the Coulombic interaction in the calculation of the material gain for a typical ZnCdSe-ZnSe quantum well structure. The enhancement for this II-VI structure is significantly larger than previously calculated for GaAs quantum wells. The intraband scattering rate used in the determination of the gain is calculated for both carrier-carrier and carrier-phonon scattering mechanisms. Our results show that the carrier-phonon scattering contribution is considerably more significant in these II-VI structures than previously calculated for III-V quantum wells and therefore is an important inclusion in the calculation of gain.

Many body effects manifest themselves in three main ways in the optical recombination spectra.[10–12] Optical transitions are broadened due to carrier scattering events. The band gap decreases (renormalisation) and the transition probability is enhanced due to the increased recombination resulting from the Coulomb attraction between electrons and holes. The room temperature gain characteristics of GaAs quantum wells have been calculated including many body effects.[10–12] These calculations show that band gap renormalisation and spectral broadening are important for the prediction of the optical gain spectra,[12] although the Coulomb enhancement has been shown to be negligible.[10] The increased exciton binding energies in II-VI materials suggests that the Coulomb interaction would be more important in these materials.

The absorption spectrum can be determined from the imaginary part of the optical susceptibility,[11] which is given by

$$\chi(\hbar\omega)=\sum_k d_k\chi_k \tag{1}$$

where

$$[\hbar\omega-E_{e,k}-E_{h,k}+i\hbar\gamma]\chi_k = -(1-f_{e,k}-f_{h,k})\left[d_k+\sum_{k'} V_s(k-k')\chi_{k'}\right] \tag{2}$$

derived using the Hartree-Fock approximation, which is reasonable at these high carrier densities and high temperatures.[11] f_c and f_v are the electron and hole Fermi functions which describe the carrier distributions at low laser intensities. V_s is the screened two-dimensional Coulomb potential within the single plasmon pole approximation.[10,11,13] d_k is the momentum dependent optical transition matrix element[14] and $E_{e,k}$ and $E_{h,k}$ are the renormalised[10] electron and hole energies at the momentum k. Setting the potential to zero in Eq. (2) gives the free carrier result, where the Coulomb interaction is neglected. In this paper, we compare the calculated gain characteristics of a 40 Å $Zn_{0.8}Cd_{0.2}Se$-ZnSe quantum well at 300 K, with and without the Coulomb interaction.

We have calculated the band structure using a 4×4 Luttinger-Kohn Hamiltonian including strain.[15] The calculations show that the bands are reasonably parabolic since the strain causes reduced intermixing of the light and heavy hole subbands. Therefore to reduce the computation time required we have used parabolic bands, the masses of which are de-

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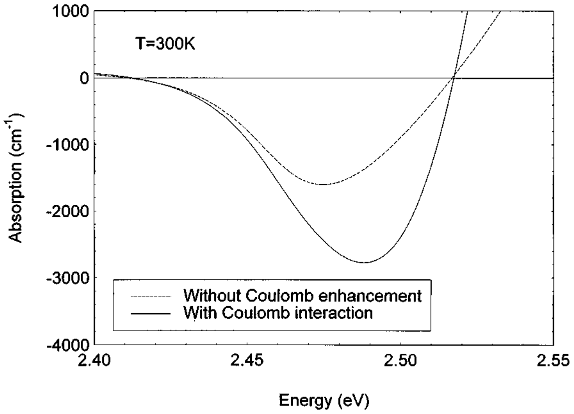

FIG. 1. Calculated gain spectra for a 40 Å $Zn_{0.8}Cd_{0.2}Se$-ZnSe quantum well calculated with and without the effect of Coulomb enhancement at a carrier density of 1.1×10^{19} cm^{-3} at 300 K.

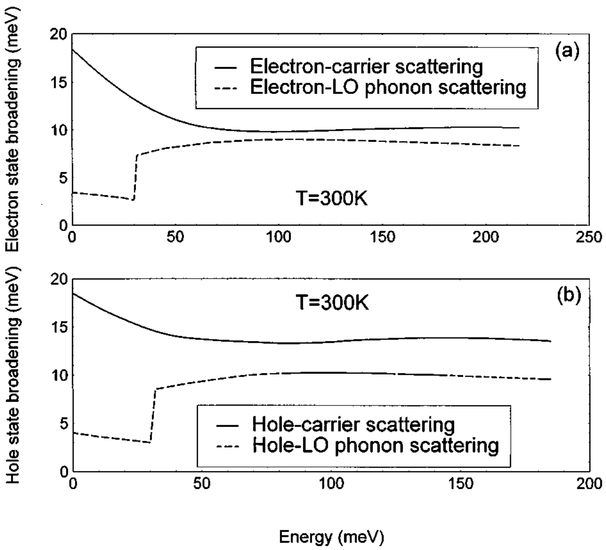

FIG. 2. The energy broadening of the electron/heavy hole state in the lowest (a) conduction and (b) valence subbands as a function of energy (relative to the bottom of the subband) at a carrier density of 1.1×10^{19} cm^{-3} at 300 K.

termined using a least square fit to the calculated subband structure (this approach was used in Ref. 5). We have not included well width fluctuations in our calculations but expect that when the well width is reduced the effect will be increasingly significant as in the case of III-V semiconductor lasers.[12] The dephasing energy, $\hbar\gamma$, is calculated using Fermi's Golden Rule for carrier-carrier[16] and carrier-LO phonon[17] scattering mechanisms. All material parameters for these calculations were taken from Ref. 18.

Figure 1 shows calculated gain spectra for a 40 Å $Zn_{0.8}Cd_{0.2}Se$-ZnSe quantum well calculated with and without the effect of Coulomb enhancement at a carrier population of 8.3×10^{18} cm^{-3} (both calculations include band gap renormalisation). The Coulomb interaction leads to significantly higher gain at a given carrier density. Haug[10] has shown that the maximum enhancement is around the transparency point, rather than at the peak of the gain spectrum; on the other hand, the enhancement in the emission spectrum which is broader than the gain spectrum occurs at its peak.

The calculation of intraband scattering rates has been described in detail in Refs. 16 and 17 where examples were given for GaAs-AlGaAs and GaInP-InP quantum wells. Using the same method we calculate the intraband scattering for the 40 Å $Zn_{0.8}Cd_{0.2}Se$-ZnSe quantum well at a temperature of 300 K. Figure 2(a) shows the energy broadening of the electron state in the lowest conduction subband as a function of energy above the bottom of the subband, at a carrier density of 8.3×10^{18} cm^{-3}. Both carrier-carrier (solid line) and carrier-LO phonon (broken line) scattering mechanisms are shown. The energy broadening of the hole state in the lowest valence subband is given in Fig. 2(b). The carrier-carrier scattering calculation includes scattering by both electron and holes from all confined subbands.[16]

Both the electron- and hole-phonon broadening curves show the characteristic "step" at the LO phonon energy, $\hbar\omega_{LO}$, due to the carrier being scattered by phonon emission above $\hbar\omega_{LO}$.[17] The broadening energies for the conduction and valence bands are very similar in magnitude due to the light in-plane hole mass (approximately equal to the electron mass) in this strained system. An important point to note is the size of the carrier-phonon broadening, especially above $\hbar\omega_{LO}$. The magnitude is comparable with the carrier-carrier energy, which is in contrast to GaInAs-InP wells[17]where the carrier-carrier (total of the electron and hole) scattering is more dominant. This is because the ZnSe optical dielectric constant is smaller than that of GaInAs. The small carrier-phonon broadening below $\hbar\omega_{LO}$ is compensated by the high carrier-carrier broadening energy at the subband edge and so the total broadening energy for electrons and holes remains reasonably constant with respect to energy. The average of the total carrier and phonon broadening for electrons and holes is used to obtain the scattering lifetime.[17] The scattering lifetime for the first electron-heavy hole transition varies from 29 fs at the transition energy to around 32 fs at higher energies, peaking at 37 fs just below $\hbar\omega_{LO}$. These lifetimes compare with the constant 25 fs lifetime required to fit experimental data in Ref. 5 for a 65 Å ZnSe quantum well. This is an important result because the gain spectra of II-VI quantum wells are often calculated using a constant lifetime of 100 fs, which is clearly too long.

Figure 3 shows the gain-current characteristics for a 40 Å $Zn_{0.8}Cd_{0.2}Se$-ZnSe quantum well calculated with and without the effect of Coulomb enhancement. Although the Coulomb enhancement increases the amount of gain at a given carrier density, it also increases the amount of spontaneous emission, therefore the spontaneous recombination current required to achieve transparency is higher. Assuming an internal scattering loss of 6 cm^{-1} as measured by Kozlov[19] for a single quantum well structure with a ZnCdSe active region and a typical confinement factor of 0.015 for a 40 Å well, we estimate the typical gain required to overcome the cavity losses for a 340 μm laser to be 3500 cm^{-1}. From Figure 3, when Coulomb enhancement is included the predicted threshold current density is 1300 A cm^{-2}, compared with 800 A cm^{-2} when the effect is neglected, an underestimate

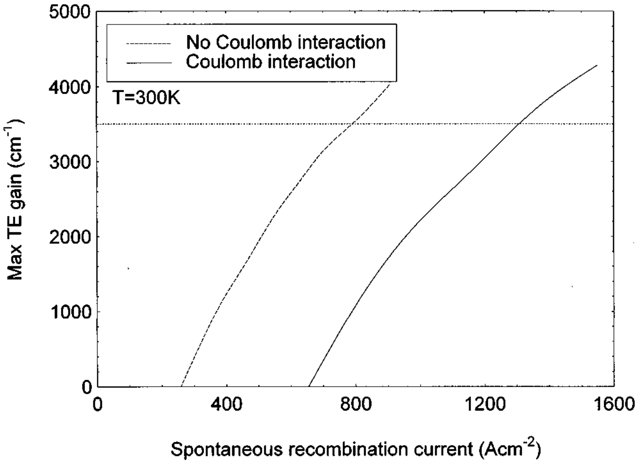

FIG. 3. Calculated gain-current characteristics for a 40 Å $Zn_{0.8}Cd_{0.2}Se$-ZnSe quantum well at 300 K, calculated with and without the effect of Coulomb enhancement.

of 40%. A value for the internal quantum efficiency is needed to predict a true threshold current density.

The injected carrier density required to achieve threshold when Coulomb enhancement is included is approximately 8.3×10^{18} cm^{-3}, compared with 1.2×10^{19} cm^{-3} when Coulomb effects are neglected. Neglecting the Coulomb interaction leads to an overestimate of the electron quasi-Fermi level by 18 meV. This is an important result because the thermal emission of electrons out of the well is exponentially proportional to the conduction band Fermi level.[20] This loss mechanism is an essential consideration in the modelling of device threshold currents especially at high temperature. In our example, the omission of Coulomb effects would lead to the overestimate of the leakage current out of the quantum well by more than a factor of 2 at 300 K (due to a difference in Fermi level of 18 meV). The calculated peak of the gain spectrum at threshold is 497 nm, but when Coulomb effects are neglected the predicted peak is 501 nm, a shift of 4 nm in the predicted laser wavelength.

In conclusion we have shown the effect of the Coulomb interaction is a very important consideration in the calculation of the gain spectra for ZnCdSe-ZnSe structures. When Coulomb effects are neglected the spontaneous emission current at threshold is underestimated by as much as 40% and the predicted lasing wavelength is overestimated by 4 nm. We also show the carrier-LO phonon scattering mechanism to be an important aspect of the calculation of gain in ZnCdSe-ZnSe quantum wells. The discrepancy in the conduction quasi-Fermi level when Coulomb effects are neglected also means that the subsequent calculation of thermally activated leakage currents is flawed.

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