NUMERICAL MODELING OF INJECTION INDUCED CARRIER CONFINEMENT IN QUANTUM-WELL (QW) STRUCTURES

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Abstract

A comprehensive band filling model including the injection induced carrier confinement effect has been developed for device simulation of QW lasers, based on self-consistently solving the Schroedinger and Poisson equations. A simplified approach has also been derived for quick evaluation in gain calculation.

I. INTRODUCTION

The Separate Confinement Heterostructure (SCH) Single Quantum Well (SQW) laser is a commonly used structure to achieve low threshold current density operation. In such a structure, as shown in Fig.1, the carriers (electrons and holes) are mainly confined by the band offsets ΔE_c and ΔE_v between QW and barriers (optical guiding layers). In real laser structures, ΔE_c and ΔE_v are often less than 0.2 eV. As the injection level becomes increasingly higher, quasi-Fermi levels are raised and carrier distributions in the barriers will increase. This carrier spill-over may becomes significant, especially in diode lasers operating at high temperature or in laser structures with low band offsets (poor carrier confinement). Generally, due to the structural difference between conduction and valence band, (e.g. electron-to-hole effective mass ratio is about 1/6 in ZnCdSe/ZnSSe based lasers), the spill-over of electrons and holes tend to be different. This will result in an internal electrostatic field which works to reduce the difference of the electron and hole distributions, leading to the modification of the band profile.

An extreme case of this kind of injection-induced carrier confinement can be found in some laser structures where one of the conduction or valence band is completely flat or even slightly type-II. In such a case, it is still possible to get some carrier localization due to the electrostatic attraction generated by space charges as demonstrated in reference[1]. In some more general cases, even with structures that have type-I band alignment, the threshold carrier density for lasing may be very high and the carrier confinement is relatively poor, as in most wide bandgap II-VI compounds based lasers. It is still necessary to evaluate this injection-induced electrostatic confinement effect in gain/threshold current calculations for device design and optimization. Also, the quantitative modeling of this effect can

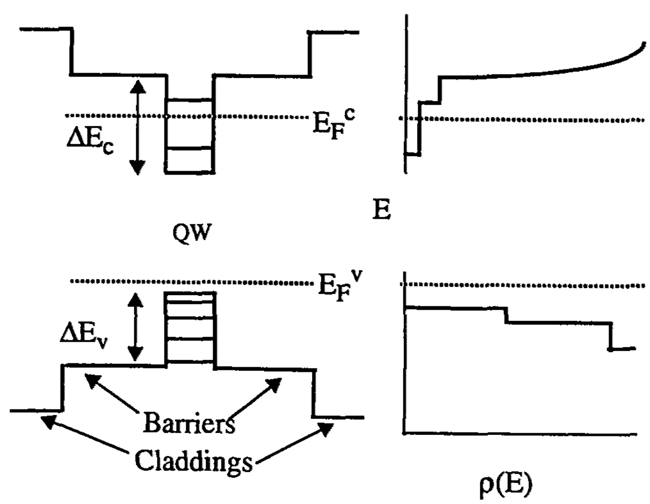

Fig.1 SCH SQW structure and density of states.

help us gain more understanding about the influence on device performance of band offset ratio $Q_c = \Delta E_c / (\Delta E_c + \Delta E_v)$, whose value for the time being is still very difficult to predict. In this paper we will present a comprehensive band filling model for a SCH SQW laser structure which including the spill-over carriers contribution.

The numerical method is based on solving the coupled set of Poisson and Schroedinger equations. An accurate picture of carrier distributions can be obtained from this comprehensive model. Based on these we then developed a simplified approach for quick evaluation of this effect in gain/threshold-current calculation through band offset ratio adjustment. The controversy on band offset ratios can possibly be clarified in this way. As an example, the numerical simulation results on a ZnCdSe/ZnSSe based laser will be presented.

II. BAND FILLING MODEL

Flat quasi-Fermi levels across the hetero-junction between QW and barrier are assumed and the carrier densities in QW and barrier regions are obtained under Fermi-Dirac distributions. The two-dimensional carrier density distribution in the z-direction can be described by

$$n(z) = k_B T \sum_i |F_{e,i}(z)|^2 \times \rho_{c,i} \times ln\left(1 + e^{(E_F^c - E_{e,i})/(k_B T)}\right),$$
$$p(z) = k_B T \sum_i |F_{h,i}(z)|^2 \times \rho_{v,i} \times ln\left(1 + e^{(E_F^v - E_{h,i})/(k_B T)}\right) \quad (1)$$

where k_B is Boltzmann constant and T is the temperature. E_F^c and E_F^v are the quasi-Fermi levels in conduction and valence band, respectively. $E_{e,i}$ and $E_{h,i}$ are the quantized energy levels, and $\rho_{c,i}$ and $\rho_{v,i}$ are the density-of-states functions of electrons and holes of the i-th subband. Here we also include those unconfined (spill-over) states in the barrier with z-direction energy higher than the band off set ΔE_c and ΔE_v. The envelope functions $F_{e,i}(z)$ of electrons and $F_{h,i}(z)$ of holes are described by Schroedinger equations:

$$\left(-\frac{h^2}{2m_e}\frac{d^2}{dz^2} + U_e(z) + V(z)\right)F_{e,i}(z) = E_{e,i}F_{e,i}(z),$$
$$\left(-\frac{h^2}{2m_h}\frac{d^2}{dz^2} + U_h(z) - V(z)\right)F_{h,i}(z) = E_{h,i}F_{h,i}(z) \quad (2)$$

For simplicity the effective masses m_e and m_h are considered constant. $U_e(z)$ and $U_h(z)$ are the conduction and valence band-edge potentials. V(z) is the electrostatic potential generated by space charge due to the imbalance of electron and hole spatial distribution, which can be described by Poisson's equation:

$$\frac{d^2}{dz}V(z) = \frac{e^2}{\varepsilon}[n(z) - p(z)] \quad (3)$$

The numerical solutions of the above problem are similar to those applied in HEMT (high electron mobility transistor) simulations, except now both electrons and holes need to be considered at the same time. The solution of Poisson's equation is based on a standard finite difference method. The solution of Schroedinger's equation follows the Numerov process as described by P. C. Chow[2]. The band profile and carrier distributions are then obtained by self-consistent iteration procedures. Based on the detailed simulations, a simplified approach has also been developed for easy incorporation into gain calculation.

III. SIMPLIFIED APPROACH FOR GAIN MODELING

In practice, it is important to have a flexible modeling program available that allows to elucidate trends in a large parameter space rather than a sophisticated procedure that generates highly accurate data for specialized situations. The injection-induced confinement effect can be incorporated into gain modeling in a simplified way. The basic feature of this approach assumes that the injection induced space charge distribution is an interface dipole sheet, and this dipole sheet only changes the built-in potential of the hetero-junction. In other words, we use the band offset Q_c as an adjustable parameter to fulfill the charge neutrality condition in both QW and barrier regions. Thus, an injection level dependent Q_c which makes the carrier densities of electrons and holes in both QW and barrier almost equal, can be derived. Based on this, we can then calculate the gain spectrum and the radiative current including the influence of barrier recombination, in a self-consistent manner. The gain/current calculations are based on the model introduced in Ref.[3] except in our case we also include the barrier recombinations.

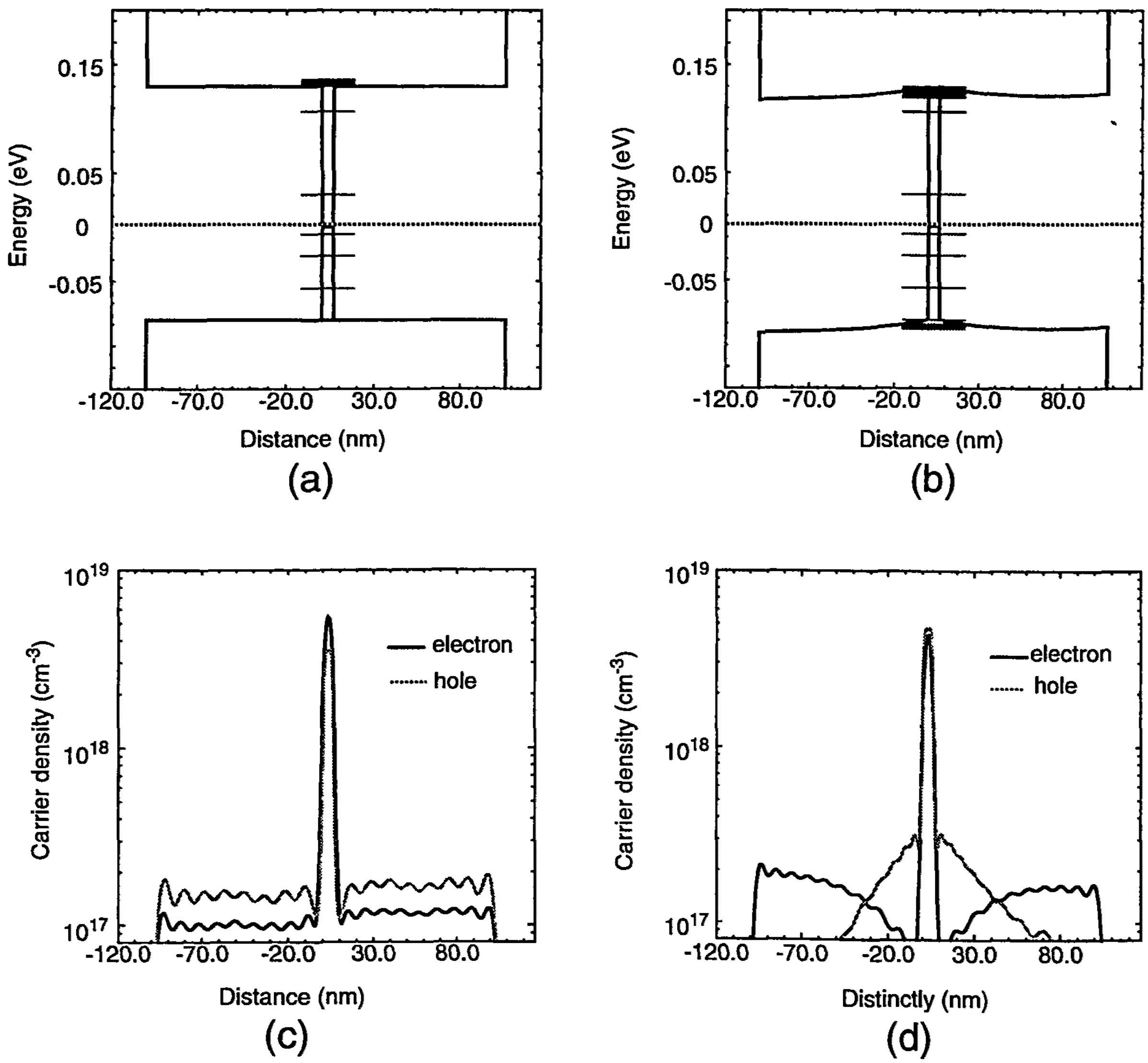

Fig.2 Band profile (without QW band gap) and carrier distribution. (a) Initial band diagram (b) Band diagram including injection induced carrier confinement (c) Unbalanced carrier distribution of configuration (a). (d) balanced carrier distribution of configuration (b).

IV. RESULTS

As an example, we consider a particular device structure (SCH SQW $Cd_{0.2}Zn_{0.8}Se/ZnS_{0.06}Se_{0.94}$ 6.5 nm QW, 100 nm barrier) to perform our numerical calculations. The injection levels is about $5x10^{18}$ cm^{-3} which is close to the threshold carrier density measured in the experiments. The initial band configuration is shown in Fig.2a, as estimated from strain effect and common anion rule. The Q_c value (refers to heavy hole band-edge) in this case is about 0.62. As we keep the total charge neutrality in the combined barrier and QW region, the locally unbalanced carrier distribution at this injection level is shown in Fig.2c, where in this particular case there are more electrons in QW and more holes in barriers. The modification of the band profile due to the locally unbalanced carrier distribution is obtained with the comprehensive model as shown in Fig.2b. The injection induced carrier confinement can be clearly observed when compared to the balance carrier distribution shown in Fig.2d.

Next we use our simplified approach to evaluate gain/threshold current relation. Here Q_c is changed to provide for the same quasi-Fermi levels as those in comprehensive model. Once this condition is satisfied, Q_c = 0.53 is obtained and the carrier distribution are found to be very close to those calculated in the comprehensive model and the charge neutrality condition in both QW and barrier region are then satisfied as shown in Fig.3. The gain and threshold current density is as calculated for Q_c = 0.53 is plotted in Fig.4. The results are very close to the value of 500 A cm^{-2} which has been observed experimentally.

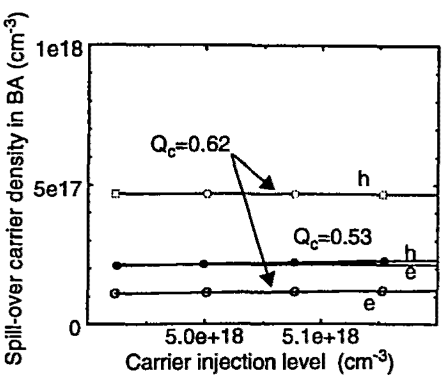

Fig. 3 Carrier spill-over under different Q_c

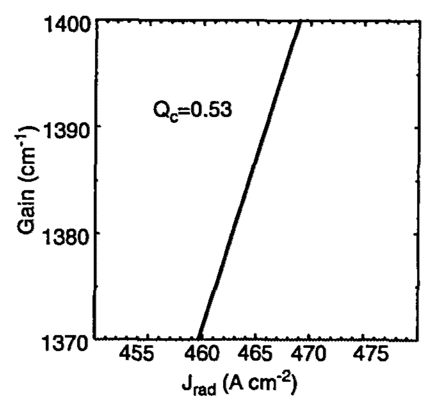

Fig. 4 Gain vs. radiative current density.

V. CONCLUSIONS

In summary, we have developed a comprehensive theoretical approach to analyze the injection induced carrier confinement and its influence on band filling process of SCH SQW lasers. A simplified approach has also been derived for quick evaluation. It has been shown that in modeling of ZnCdSe/ZnSSe based diode laser, the method can give satisfied explanation of observed results.

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