THEORETICAL PERFORMANCE OF MID-INFRARED BROKEN-GAP MULTILAYER SUPERLATTICE LASERS

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ABSTRACT

We present calculations of the intersubband absorption and Auger recombination rate of superlattices based on the InAs/GaInSb material system involving more than two layers in the repeating unit cell and strain balanced to match the GaSb substrate. We demonstrate theoretically the presence of final-state optimization in a 4.0 µm strain-balanced broken-gap superlattice. This system’s band structure is optimized not only at the band edge, where the valence density of states has been reduced, but also at resonance energies, where reside final states for Auger and intersubband processes. The spectral structure of the intersubband absorption, which for some wavelengths near the lasing wavelength can exceed 500 cm⁻¹ at lasing threshold, has been considered when designing this active region. Fortunately, final-state optimized designs which minimize Auger recombination tend to minimize intersubband absorption as well. The effectiveness of final-state optimization is evaluated by considering band structures with identical band edge structure, but different final-state structure.

INTRODUCTION

Recent work on mid-infrared lasers can be separated into two rough categories according to whether the light is generated in an interband[1-7] or intersubband[8] transition. The dominant non-radiative transition for the second type occurs via electron-phonon scattering, and has a typical timescale of picoseconds. The dominant non-radiative transition for interband lasers, by contrast, has a timescale of nanoseconds, and is due to carrier-carrier (Auger) scattering. We will focus here on the issues associated with improving interband lasers in the mid-infrared through band-structure engineering of a strain-balanced broken-gap superlattice active region.

Optimizing band structures is a key challenge in the design of mid-infrared lasers. Considerable optimization is possible through changing the band structure at the band edges. By introducing strain, the valence density of states can be reduced, thus decreasing the threshold carrier density \( n_{th} \). Reduction of \( n_{th} \) leads to a reduced intervalence absorption (which is proportional to \( n_{th} \)) and Auger rate (proportional to \( n_{th}^3 \) at low density). We will refer to this form of band structure optimization as band-edge optimization.

Our focus will be on final-state optimization, a term which refers to reducing the availability of final states for Auger processes and intervalence absorption. For a fixed density these designs reduce intervalence absorption and Auger rates. Reduction of intervalence absorption indirectly reduces \( n_{th} \), but reduction of the Auger rate does not. Reduction of the Auger rate does, however, reduce the more important physical quantity \( J_{th} \), the threshold current density. Since a bulk system has neither band-edge nor final-state optimization we emphasize that demonstrating a suppressed Auger rate relative to a bulk system does not necessarily mean there is final-state optimization.

A particular example of a system exhibiting final-state optimization will be presented. Its 300K Auger rate is a factor of two smaller than another optimized type II system with the same band gap but without final-state optimization at 300K[3]. We then explore the sensitivity of this type of band structure to changes which affect the final states while leaving the band-edge electronic structure unchanged.

We continue by addressing possible problems associated with final-state optimization, such as vertical transport in a system with a highly quantized band structure. We will conclude with a system which should have acceptable transport properties, but which maintains the high degree of structure in its final states for Auger processes and intersubband transitions.

THEORY

Calculations of the band structure including non-parabolicity, and the K-dependent optical matrix elements, were performed with a superlattice K·p technique (see references in Ref. 9). Our confidence in this type of calculation is bolstered by exceptional agreement with measurements on a type II superlattice multiple quantum well[10]. The radiative and non-radiative recombination rates were then calculated with the procedure described in Ref. 11.

RESULTS

Figure 1 shows a structure which exhibits final-state optimization, 15Å InAs, 25Å In<sub>0.40</sub>Ga<sub>0.60</sub>Sb, 15Å InAs, and 39Å Al<sub>0.38</sub>In<sub>0.28</sub>Ga<sub>0.42</sub>As<sub>0.50</sub>Sb<sub>0.50</sub>. The band edges are shown in Fig. 1(a) and the band structure in Fig. 1(b). Final-state optimization is possible in

![Figure 1](image-url)

Figure 1: (a) Band offsets for the strain-balance broken-gap superlattice described above. (b) Band structure in the growth direction (K<sub>∥</sub>) and in-plane direction (K<sub>⊥</sub>). The resonance energies in the superlattice are indicated, as are the valence and conduction edges.
this structure because of the large range in band edges, from an energy gap $E_g$ above the superlattice conduction band to $E_g$ below the superlattice valence band edge. This range of band edges produces structure in the band structure at $E_g$ above the superlattice conduction minimum and at one $E_g$ below the superlattice valence band. Resonance energies are indicated in gray. Final states for Auger processes must lie above the $2E_g$ line in the conduction band (for electron Auger processes) or below the $-E_g$ line in the valence band (for hole Auger processes). In electron Auger processes the energy from the recombining electron-hole pair is transferred to an electron; in hole Auger processes it is transferred to a hole.

These structures in the conduction and valence band produce gaps in the intersubband absorption as shown in Fig. 2(a). The gap is somewhat smaller than either the zone-center or growth-direction zone-edge LH1—LH2 gap because transitions elsewhere in the Brillouin zone also contribute. Transitions which narrow the gap occur at the growth-axis zone boundary at finite in-plane momentum. This gap is placed around the peak of the gain region (the gain is shown in Fig. 2(b)). Thus $n_{th}$ is lower, for the intersubband absorption does not need to be overcome. In contrast, a type I system[7] (whose intersubband

![Figure 2](image_url)

Figure 2: (a) Intersubband absorption for the strain-balanced broken-gap superlattice for several carrier densities, showing a pronounced gap between transitions associated with the LH1 and LH2 subbands. (b) Gain spectrum for the same structure and the same densities. The peak of the gain is in this gap in the intersubband absorption. (c) Intersubband absorption for a type I system[7], 80Å InP$_{0.24}$As$_{0.76}$/80Å InAs$_{0.86}$Sb$_{0.14}$. The densities plotted are the same as in (a) and (b). (d) Gain spectrum for the type I system, showing a smaller peak gain than the strain-balanced broken-gap superlattice.
absorption is shown in Fig. 2(c) and whose gain is shown in Fig. 2(d)) has hundreds of cm⁻¹ of intersubband absorption at the gain region, which increases n_{th}. In addition, since the intersubband absorption increases with n, the differential gain is much larger with the superlattice of Fig. 1 than that associated with Fig. 2(c,d).

Lasers with this type of active region[9] were grown and lased under optical pumping at room temperature. Possible problems with vertical transport will be addressed later in this article. A device with a strain-balanced broken-gap superlattice active region similar to that described above, but with a band gap of 5.2 μm, also lased under optical pumping up to 185K, making it the longest-wavelength III-V interband laser to date[12].

The spectrum of this 5.2 μm laser was of some interest, and is shown below in Fig. 3 for several temperatures. There is a “hole” in the spectrum at intermediate temperatures. It does not originate with an atmospheric absorption line, for the hole moves with temperature. The movement of the line with temperature roughly corresponds to the expected movement of an intervalence absorption feature. This hole, therefore, may be due to an intervalence absorption peak which has unfortunately ended up interfering with the gain region. The characteristic temperature (T_c) of this laser was 37K from 40K to 140K.

![Spectra for several temperatures of a 5.2 μm (at 185K) laser.](image)

The Auger recombination has been calculated for the system of Fig. 1, and is shown in Fig. 4(a,b) as a function of density at T = 300K. The low-density Auger coefficient is C = 2.5 × 10⁻²⁷ cm⁶/s, which is four times smaller than that of InAs[13], which has a band gap 40 meV larger. The calculations are performed including superlattice Umklapp processes, which have been ignored in the past and are insignificant in bulk semiconductors[14]. Here the difference between the calculation with Umklapp and without Umklapp is more than a factor of two.

In Fig. 4(b) the rate per carrier is plotted versus n² to show clearly the deviation from n². Although a sub-quadratic behavior has been predicted at high densities[15,16], this is the first realistic calculation (i.e., which does not assume T = 0K[15] or rely on the density dependence of the “most-probable transition”[16]). The deviation occurs at approximately the density where the valence band becomes degenerate (the conduction band is degenerate for the entire range of densities considered here). This correlation implies that the rate is dominated by hole Auger. The agreement with experimental measurements (see article by J. T. Olesberg, et al., in this volume) is exceptional.
Figure 4: (a) Non-radiative recombination rate for the strain-balanced broken-gap superlattice, calculated without (circles) and with (diamonds) Umklapp processes. The solid line fits the calculations at low densities, and is an $n^2$ extrapolation to higher densities. (b) Same calculations plotted versus $n^2$ to better indicate the deviation of the calculations from $n^2$.

The dominant hole and electron processes are shown below in Figs. 5(a,b) respectively. The most probable holes are indicated with open circles, and the most probable electrons are indicated with filled circles projected onto the in-plane direction of the band structure of the strain-balanced broken-gap superlattice. The band edges and the resonance energy are indicated by dashed lines. A guide to the importance of Umklapp processes is the relative size of the typical in-plane momentum transfer to the Brillouin zone width in the growth direction. For this system it is clear that the Brillouin zone width is smaller than this typical momentum transfer.

As mentioned before, comparison with a bulk system’s Auger rate is not a good test of final-state optimization for the bulk system does not have band-edge optimization. Fig. 6, below, shows a comparison of the Auger rate per carrier for the strain-balanced broken-gap superlattice versus a T2QW structure[3] at the same wavelength. The difference in rate is about a factor of two. Since the T2QW structure is expected to have approximately the same band-edge optimization as the strain-balanced broken-gap superlattice, the Auger rate difference must originate from final-state optimization.

We now explore the importance of final-state optimization in influencing Auger rates. Shown in Fig. 7(a) are the most probable transitions in a 3.7 μm strain-balanced broken-gap superlattice[9] at 77K. Our focus is entirely on the dominant Auger process: hole Auger. Momentum conservation constraints require the electrons at 77K to have excess
Figure 5: (a) Most probable transitions for hole Auger in the strain-balanced broken-gap superlattice. The arrows indicate the single most probable transition. (b) Most probable transitions for electron Auger in the strain-balanced broken-gap superlattice.

Figure 6: Comparison of the Auger rate per carrier between the strain-balanced broken-gap superlattice and a T2QW structure at the same wavelength.
energy relative to the conduction minimum of approximately 30 meV, corresponding to \( \sim 4k_B T \). Since the occupation factors are proportional to \( \exp(-E/k_B T) \), this energy difference produces a reduction in the occupation factor, and thus in the hole Auger rate, of two orders of magnitude.

Our procedure is to take the band structure shown in Fig. 7(a) and manually shift the fourth, fifth, and sixth valence subbands from the valence edge (shown as dashed lines) and observe the effect on the carrier lifetimes. As the bands are shifted up more states at zero in-plane momentum become accessible as final states for Auger processes. We show in Fig. 7(b) the most probable transitions for the same situation as Fig. 7(a), but with the band shifted 90 meV up. It is evident that the electrons in the conduction band which were 30 meV above the band edge are now at the band edge. Hence the final-state optimization has been removed. Fig. 7(c) shows the carrier lifetime as a function of the energy shift of the bands towards the band edge. The difference in the lifetime between the optimized case of Fig. 7(a) and the unoptimized case of Fig. 7(b) is over two orders of magnitude.

In Fig. 8(a,b,c) the situation at 300K is shown. Due to the marked sensitivity of the Auger rate on band gap the differences in the band structure at 77K and 300K are ignored; we use the 300K band structure for both carrier temperatures. Whereas the non-equilibrium carriers were quite concentrated at the zone center at 77K, here they are substantially more spread out. In addition, the non-equilibrium electrons involved in the most probable transitions are located at the conduction band minimum. Hence the contribution of final-state optimization to reducing the 300K Auger rate in this structure appears small. This is supported by Fig. 8(c), which shows the lifetime as a function of the band shift. We note that the 4.0 \( \mu \)m structure mentioned above as having final-
state optimization roughly corresponds on Fig. 8(c) to an energy shift of $-30$ meV, which indicates an Auger rate suppression of a factor of 2.

We now address the issue of vertical transport in these structures. Since the valence band structure has little dispersion up to energies greater than the band gap, one might be concerned about vertical hole transport. This issue may be avoided by designing a system which allows transport near the band edge, but maintains the quantized structure at the resonance energies. Such a structure is shown in Fig. 9. Fig. 9(a) shows the band edge diagram for a superlattice injector into a superlattice well. The superlattice well has a band structure (shown in Fig. 9(b)) similar to the strain-balanced broken-gap superlattices described above. The barrier, however, is designed to allow for electron and hole transport at certain energies (indicated on the band structure diagram in Fig. 9(c) with gray shading), but to prevent such transport at the resonance energies. Thus a minigap of the superlattice injector is positioned near the resonance energies. The combination of the two pieces of the structure yields the band structure shown in Fig. 9(d). Transport is allowed for the highest valence subbands, except for the very top one, but is difficult for subbands near the resonance region. With such a design we can have quantized electronic structure at the resonance energies, but dispersive structure closer to the band edges.

CONCLUSIONS

The intersubband absorption and Auger rates have been calculated for strain-balanced broken-gap superlattices in the mid-infrared. Final state optimization of a 4.0 $\mu$m structure has been demonstrated by comparison with a structure with band-edge optimization. The sensitivity of final-state optimization to band location and temperature has been explored. A new design is proposed which allows for optimized intersubband absorption and Auger rates, and is expected to have good vertical transport.
Fig. 9: (a) Band edges for a superlattice injection region and well (gray). (b) Growth-direction band structure of repeating well units. (c) Same as (b) but for the injector/barrier. Transport is allowed for those energies with dispersive subbands (indicated by gray). (d) Band structure of combination, showing dense states right below the valence maximum and gaps at the resonance energies in the valence and conduction bands.
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