Optimization of MWIR Type II Superlattices for Infrared Detection

C. Grein and M.E. Flatté
EPIR Technologies, Bolingbrook, IL 60440

ABSTRACT
Type II superlattices (SLs) offer a broad range of design degrees of freedom to help optimize their properties for infrared detection. Under the AFRL STEPS contract, we focus on mid-wavelength infrared (MWIR; 2-5 µm bandpass) Type II structures with two-layer InAs/GaInSb and four-layer “W-structure” InAs/GaInSb/InAs/AlInGaAsSb SL periods. We consider details of the electronic band structures that reduce Auger recombination rates in p-type SLs specifically by affecting the density of final states available to one of the involved carriers. This work assesses the potential impact of final state optimizations on 5 µm band gap SLs in the 200-225 K operating temperature range.

Keywords: Type II superlattice, infrared, detector, Auger recombination

1. INTRODUCTION
High quality, high operating temperature infrared photodiodes typically have their sensitivity limited by Auger recombination. Type II SLs offer the possibility to design features into their electronic band structures that reduce the rate of Auger recombination, for example by reducing the density of available final states. Designing a SL to exhibit Auger suppression via final state optimization becomes more challenging as the SL band gap increases due to the increasing number of SL subbands that exist in critical regions of the electronic band structure. MWIR SLs are therefore particularly challenging to optimize. Our previous work\(^1\) considered an MWIR SL for laser applications and found that final state optimization to suppress Auger recombination can produce pronounced recombination lifetime improvements at 77 K but has little effect at 300 K. This work considers a slightly longer cutoff wavelength in the MWIR, operating temperatures in the 200-225 K range and carrier distributions representative of infrared detectors rather than lasers. We undertake a similar theoretical exercise in terms of subband shifting to assess the possible impact of band engineering on tuning Auger recombination rates in MWIR detectors.

2. ELECTRONIC STRUCTURE
We designed a superlattice that has a 5 µm bandgap wavelength at 200 K. The calculations of the electronic band structure are based on a 14-band bulk basis for the III-V constituents of the superlattice, and an envelope-function-based superlattice \(K\cdot p\) formalism. The superlattice is considered to be a highly anisotropic periodic structure. The zone-center states are calculated in Fourier space using a 14-band basis for the envelope functions. The need to rely on a 14-band basis rather than the more common 8-band basis arises because of the sensitivity of the optical and electronic properties to the electronic structure in the secondary regions of the band structure. Errors inherent in the 8-band model become significantly more pronounced as the states one is interested in become farther from the band edge. This is particularly relevant in MWIR structures.

The use of Fourier space to solve the envelope function equations at the zone center avoids the issues associated with matching conditions at sharp interfaces and also provides a sensible way to choose a balanced basis set for the superlattice \(K\cdot p\) calculations. Momentum matrix elements are then evaluated among these superlattice states, and a \(K\cdot p\) calculation using entirely the superlattice states is performed.
3. COMPUTATION OF RECOMBINATION RATES

Auger recombination rate calculations, which are computationally more intensive, require additional approximations and are thus characteristically less accurate than optical properties. The highly nonparabolic band structures and momentum matrix elements are used directly as input for the computation of Auger lifetimes. They are input into the Auger rate computations in the form of look-up tables with a mesh spacing of 0.002 Å⁻¹. The principal methods employed are discussed in ref. 2, and have been extended to include the effects of superlattice Umklapp processes. Umklapp processes are negligible in bulk direct gap systems. However, due to the large size of the superlattice unit cells and hence the small size of reciprocal lattice vectors in the growth-axis direction, Umklapp processes have shown to contribute approximately half of the total rate of Auger recombination in superlattices. The transition matrix elements are evaluated using a statically screened Coulomb interaction and first order Kₚ formalism, and evaluated with the standard van Roosbroek-Shockley expression multiplied by Humphreys correction factor to account for photon recycling (assuming an absorption coefficient of 1000 cm⁻¹ and device thickness of 10 µm).

Radiative lifetimes are also computed employing directly the band structures and matrix elements from the 14 band Kₚ formalism, and evaluated with the standard van Roosbroek-Shockley expression multiplied by Humphreys correction factor to account for photon recycling (assuming an absorption coefficient of 1000 cm⁻¹ and device thickness of 10 µm).

Defect-mediated recombination is not included in the calculations. Actual lifetimes are expected to be shorter than those predicted here due to the presence of recombination-mediating defects.

4. RESULTS

Ref. 1 focused on MWIR superlattices for laser applications and hence considered high and equal concentrations of injected electrons and holes. This paper focuses on MWIR detectors; hence we consider a p-type doping level of 5x10¹⁵ cm⁻³ with no compensating donors. The superlattice was designed to suppress hole-hole Auger recombination through appropriate band structure engineering. This involves reducing the density of final states for Auger transitions by the appropriate positioning of superlattice subbands, hence reducing the probability of their occurrence. The designed “W” structure superlattice is shown in Fig. 1. It has layer compositions and thicknesses 28.4 Å InAs/24 Å Ga₀.₉₉In₀.₁₀Sb/28.4 Å InAs/40 Å Al₀.₃₀In₀.₂₈Ga₀.₄₂As₀.₅₀Sb₀.₅₀, and a 248 meV (5 µm) band gap at 200 K. Superimposed upon the band structure in the figure are the positions of the initial state holes and electrons computed to constitute the approximately 400 most probable Auger transitions. The subbands labeled “7,8” are too high in energy to support final hole states in Auger transitions involving the scattering of two holes in the subbands labeled “9,10”. The dominant final hole states in the valence band are in the subbands labeled “5,6”, with the subbands labeled “3,4” also providing some final states. The latter are less probable than “5,6” due to the requirement for the associated initial state electrons to be present in conduction subbands “11,12” at quite high energy (lower occupation probability).

To test the sensitivity of the lifetimes to band engineering, our procedure was to take the band structure shown in Fig. 1 and artificially shift the valence subbands 5, 6, 7 and 8 up and down in energy and observe the effect on the carrier lifetimes. As the bands are slightly shifted upward, more states near zero in-plane momentum become accessible as final states for Auger processes and hence the lifetime shortens. We show in Fig. 2 the approximately 400 most probable transitions for the same situation as Fig. 1, but with the four subbands shifted up by 50 meV. Immediately evident in Fig. 2 is that the electrons (solid circles) in the conduction band that were present in energy up to about 325 meV above the valence band edge in Fig. 1 are now in the range of up to 300 meV above the valence band edge. The higher occupation probabilities of the electrons in Fig. 2 relative to Fig. 1 lead to shorter Auger lifetimes.
Figure 1: Computed electronic band structure of a 28.4 Å InAs/24 Å Ga_{0.85}In_{0.15}Sb/28.4 Å InAs/40 Å Al_{0.95}In_{0.05}As_{0.78}Sb_{0.50}
superlattice at 200 K. The electrons (solid circles) and holes (hollow circles) involved in the (roughly) 400 most probable hole-hole
Auger transitions at 200 K and p = 5 x 10^{15} cm^{-3} are also shown.

Figure 2: Same electronic band structure as in Fig.1 except subbands 5, 6, 7 and 8 have been artificially shifted up by 50 meV. The
electrons (solid circles) and holes (hollow circles) involved in the (roughly) 400 most probable hole-hole Auger transitions at T=200
K and p = 5 x 10^{15} cm^{-3} are also shown.
The computed hole-hole-Auger lifetimes at T=200 and 225 K are plotted in Figure 3 as a function of the subband shift. The 200 K electronic bands structure and matrix elements were employed for the lifetime calculations at both temperatures. Thus any differences in lifetimes at the two temperatures are a consequence of the changes in occupation probabilities associated with temperature and not with shifts of energy states. We see that the designed structure (zero shift of subbands 5, 6, 7 and 8) is near-optimal, but indeed a superior design would have been realized had one been able to shift the four subbands down by 25 meV. A major conclusion from Fig. 3 is that the sensitivity of the lifetime to the shift implies that final state optimization plays a significant role in the design of 5 µm Type II superlattices at 200-225 K. Note that the longest to shortest lifetime ratio in the -150 to +50 shift range is smaller for T=225 K than T=200K, indicating the weaker (though still significant) impact of final state optimization as temperature is increased. The lifetime increases rapidly for very large positive or negative shifts (less than -150 meV and greater than +50 meV) since these shifts put subbands 5, 6, 7 and 8 into regions where they can no longer contribute to hole-hole Auger transitions.

The radiative lifetime is unaffected by the subband shifts. It is 1.7x10^{-4} s at 200 K and 2.1x10^{-4} s at 225 K. Note that photon recycling is included in these estimates.

The 200 K optical absorption coefficient of the superlattice with unshifted subbands is plotted in Figure 4. Thanks to the “W” structure, the optical absorption onset is quite rapid, peaking at approximately 2500 cm^{-1}. Features at higher energies in the spectrum are optical critical points involving deeper subbands. For example, the peak at 520 meV corresponds to absorption transitions near zone center from valence states in subbands 5 and 6 to conduction subbands 11 and 12.
SUMMARY

The principal conclusion of the above work is that Auger final state optimization is a viable tool for tuning the probability of hole-hole Auger transitions in 5 µm Type II superlattices at 200-225 K operating temperatures. For a near-optimal design, the hole-hole Auger lifetime approximately changes by a factor of 2 to 2.5 for a 25 meV shift of subbands that provide Auger final states. The Auger coefficients range from $8.8 \times 10^{-28}$ to $5.8 \times 10^{-27}$ cm$^6$/s depending on the subband shifts.

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REFERENCES