Estimates of Impact Ionization Coefficients in Superlattice-Based Mid-Wavelength Infrared Avalanche Photodiodes

C.H. Grein1, K. Abu El-Rub1,2, M.E. Flatté3, and H. Ehrenreich4
1 Microphysics Laboratory and Department of Physics, University of Illinois at Chicago, Chicago, IL 60607-7059
2 Department of Physics, Jordan University of Science & Technology, Irbid-Jordan
3 Optical Science and Technology Center and Department of Physics and Astronomy, University of Iowa, Iowa City, IA 52242
4 Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138

ABSTRACT

We describe band engineering strategies to either enhance or suppress electron-initiated impact ionization relative to hole-initiated impact ionization in type II superlattice mid-wavelength infrared avalanche photodiodes. The strategy to enhance electron-initiated impact ionization involves placing a high density of states at approximately one energy gap above the bottom of the conduction band and simultaneously removing valence band states from the vicinity of one energy gap below the top of the valence band. This gives the electrons a low threshold energy and the holes a high one. The opposite strategy enhances hole-initiated impact ionization. Estimates of the electron ($\alpha$) and hole ($\beta$) impact ionization coefficients predict that $\alpha/\beta >> 1$ in the first type of superlattice and $\alpha/\beta << 1$ in the second type.

INTRODUCTION

Strained-layer superlattices may hold promise as high gain, low noise avalanche photodiodes (APDs) with considerable spectral agility. The ability to engineer the electronic structure of superlattice APDs provides new flexibility to enhance the performance of superlattice-based APDs over those based on bulk semiconductors. One of the proposed methods to enhance the hole impact ionization coefficient ($\beta$) in a superlattice relative to that of electrons ($\alpha$) is to engineer a resonance into its valence band structure. Specifically, the idea is to place a valence band with a large density of states one energy gap below the top of the valence band. This band is expected to provide a large number of hot holes to initiate impact ionization transitions under the high field operating conditions of an avalanche photodiode. This is expected to lead to hole-to-electron impact ionization coefficient ratios $\beta/\alpha$ very different from one, and hence low noise performance. Alternatively, a high density of states conduction band may be placed one energy gap above the bottom of the conduction band in order to enhance the electron impact ionization coefficient. An additional benefit of superlattice-based APDs is that the $\beta/\alpha$ ratio can be optimized over a wide wavelength range, providing greater spectral agility than bulk semiconductor designs. The combination of spectral agility with low noise performance at high gains may provide a substantial improvement in the operational properties of APDs. To test the above ideas and to design superlattices that have $\beta/\alpha$ ratios as different as possible from one, we have performed calculations of superlattice electronic band structures, impact ionization rates, and impact ionization coefficients.
COMPUTATIONAL METHODS

The superlattice electronic band structures were computed employing a 14-band superlattice K·p formalism [1]. Input parameters are energy levels, matrix elements, effective masses, g-factors, deformation potentials, elastic constants and lattice constants of the bulk constituents, and valence band offsets between layers. The employed parameters are mainly extracted from ref. [2] and are fully reported in [1]. The bands of the bulk systems were also computed employing the superlattice K·p formalism, treating it as a superlattice with extremely thin barrier layers. This formalism has proven to be very accurate in the calculation of the optical properties of similar type-II multilayer structures [3].

The methodology employed to compute impact ionization rates in superlattices follows the methods we previously employed to compute Auger recombination rates, the time reverse of impact ionization, in superlattices [4]. Consider hole-initiated impact ionization (the expressions for electron-initiated impact ionization are similar).

The total impact ionization rate \( R_B(n,K_{2'}) \) for a hot hole in band \( n \) with wave vector \( K_{2'} \) is obtained from Fermi's Golden Rule [5],

\[
R(n, K_{2'}) = \frac{2\pi}{\hbar} \sum_{if} |V_{if}|^2 P(1, 1', 2, 2') \delta(E_f - E_i),
\]

where \( i \) denotes the initial states 1 and 2 for the two involved electrons; \( f \) denotes the electrons’ final state 1’ (state 2’ is not summed over since it is the state of the hot hole before the impact ionization transition); \( V_{if} \) is the matrix element of the screened Coulomb potential interaction between electrons 1 and 2; \( P(1, 1', 2, 2') \) is a statistical weight function giving the occupation probabilities for the involved states; and \( E_i \) and \( E_f \) are the total energies of the initial and final states, respectively.

The matrix element \( V_{if} \) in (1) is expressed in terms of Slater determinental superlattice states as

\[
V_{if} = \int d^3 r_1 d^3 r_2 \phi^*_i(r_1) \phi^*_f(r_2) \Delta_{21} - \phi^*_f(r_1) \phi^*_i(r_2) \Delta_{12} \frac{e^2}{\epsilon |r_1 - r_2|} \phi_i(r_1) \phi_f(r_2),
\]

where \( \Delta_{21} = \Delta_{12} = 1 \) when electrons 1 and 2 have the same spin; \( \Delta_{21} = 1 \) and \( \Delta_{12} = 0 \) when electrons 1 and 2 have opposite spin which is preserved in the transition; \( \Delta_{21} = 0 \) and \( \Delta_{12} = 1 \) when electrons 1 and 2 have opposite spin which is changed in the transition; \( \lambda \) is the reciprocal screening length, approximated by the Debye form [6] \( \lambda = (4\pi^2 [n + p]/\epsilon kT)^{1/2} \), where \( n \) and \( p \) are the electron and hole concentrations; and \( \epsilon \) is the static dielectric constant of the barrier layers. The superlattice wave functions are expanded in the \((L, K)\) basis:

\[
\phi_L(K, r) \equiv \langle r | LK \rangle = \frac{1}{\sqrt{V}} \sum_G C_L(K, G) e^{i(K+G)r},
\]

where \( K \) and \( G \) are the sets of superlattice wave vectors and reciprocal lattice vectors, respectively.

After substituting (3) into (2), the integrals over \( r_1 \) and \( r_2 \) are performed analytically. Umklapp processes are included in the summations over the \( G \)s. In analogy with the work of Antoncik and Landsberg [7], first-order superlattice K·p perturbation theory is employed to evaluate the overlaps of the superlattice (SL) wave function expansion coefficients \( C_L(K, G) \) at different points in \( K \) space. This permits the square of the screened Coulomb matrix element to be expressed in terms of SL momentum matrix elements,
\[
|V_{ij}|^2 \equiv \frac{384\pi^2 e^4 h^4}{e^3 m^4 V^3} \frac{\beta_{HH1,c}(K_1, K_1) \beta_{HH2,n}(K_2, K_2)}{[\lambda_i^2 + 1 K_1 - K_1, \vec{i}^2]^2} \delta(K_2 - K_2 + K_1 - K_1),
\]

where \( \beta_{LL'}(K, K') = \langle L'K'|(K-K')\cdot p|LK \rangle^2/(E_L(K')-E_L(K))^2 \) and \( m \) is the free electron mass. Electron 1 is initially in heavy hole band \( HH1 \), electron 2 is initially in heavy hole band \( HH2 \), and \( C \) denotes the conduction band state that electron 1 ionizes to. The average over spins, involving summing over all possible terms involving different combinations of \( \Delta_{12} \) and \( \Delta_{21} \), has been approximated in a manner similar to that described by Sugimura [8], resulting in a possible error in \( |V_{ij}|^2 \) of \( \pm 33\% \).

The statistical weight function \( P(1,1',2,2') \) provides the appropriate weight for the impact ionization transitions. The impact ionization rate is proportional to the probability of finding electrons in states \( K_1 \) and \( K_2 \), the probability of finding state \( K_1 \) unoccupied, and the probability of finding a hole in state \( K_2 \), namely

\[
f_n(K_1) f_n(K_2) f_p(K_1) f_p(K_2), \tag{5}
\]

where \( f_n \) and \( f_p \) are electron and hole distribution functions respectively.

Inserting (4) and (5) into (1) yields

\[
R(n, K_2) = \frac{384\pi^2 e^4 h^4}{e^3 m^4 V^3} \sum_{C,HH1,HH2} \int d^3 K_1 d^3 K_2 f_n(K_1) f_n(K_2) f_p(K_1 + K_2 - K_2) \cdot \frac{\beta_{HH1,c}(K_1, K_1 + K_2 - K_2) \beta_{HH2,n}(K_2, K_2)}{[\lambda_i^2 + 1 K_1 - K_1, \vec{i}^2]^2} \delta(E_C(K_1 + K_2 - K_2) + E_n(K_2) - E_{HH1}(K_1) - E_{HH2}(K_2)), \tag{6}
\]

where \( K_1 \) has been integrated over to eliminate the crystal momentum conserving delta function, \( E_C \) denotes the band energies in the conduction bands, and \( E_{HH} \) denotes the band energies in the heavy hole bands.

The total impact ionization rate as a function of the hot hole’s energy \( E \) and band index \( n \) is given by

\[
R(n, E) = \frac{\int d^3 K_2 R(n, K_2) \delta(E - E_n(K_2))}{\int d^3 K_2 \delta(E - E_n(K_2))}. \tag{7}
\]

The fundamental definition of the hole-initiated impact ionization coefficient in a thick multiplication region is

\[
\beta = \frac{1}{v_{dh}} \sum_n \int f_o(E) R(n, E) g(E) dE,
\]

where \( f_o(E) \) is the hole distribution function, \( g(E) \) is the density of states, \( n \) sums over valence bands, and \( v_{dh} \) is the average hole drift velocity. A similar expression exists for the electron-initiated impact ionization coefficient \( \alpha \).

We next describe the numerical methods employed to evaluate each of the functions appearing in eqn. (8). The density of states function \( g(E) \) is easily calculated directly from the \( Kp \) bands and hence will not be discussed further. One of the principal challenges is to compute the total impact ionization rate (7) accurately. The band energies \( E_n(K) \) and momentum matrix elements \( \langle L'K'| (K-K') \cdot p |LK \rangle^2 \) (appearing in the \( \beta_{LL'}(K,K') \) terms) are computed employing the superlattice \( Kp \) method and stored in look-up tables with a resolution of 0.002 Å\(^{-1}\) in \( K \)-space. The three-dimensional \( K \)-space integrals are re-expressed in terms of cylindrical coordinates \( K_1 \).
and $K_\perp$ along the in-plane and growth-axis directions, respectively. The energy conserving delta-function in (2) is evaluated by fitting a local parabolic approximation to growth-axis dispersion of $E_C(K)$ and analytically performing the $K_\perp$ integral (with the added approximation that the HH1 band has no dispersion in the growth-axis direction). One additional integral can be performed analytically due to rotational invariance in the in-plane direction. The remaining 7 one-dimensional K-space integrals are evaluated employing an adaptive-mesh Monte Carlo algorithm [9].

A second major challenge is the computation of the hot carrier distribution functions, $f_d(E)$, and drift velocities $v_d$. High field transport in the superlattices was modeled employing a Monte Carlo program to solve the Boltzmann transport equation. The employed program performs the time evolution of the position, k-state and energy of a single particle that starts at zone center at the beginning of the simulation. Actual superlattice bands extracted from 14-band superlattice $K\cdot p$ computations are employed in the form of look-up tables. Carrier scattering rates are computed including the following mechanisms: (i) intraband acoustic phonon absorption and emission, (ii) intraband optical phonon absorption and emission, (iii) interband optical phonon absorption and emission, (iv) impact ionization, and (v) ionized impurity scattering. The phonon and impurity scattering rates are calculated using the expressions for parabolic bands found in ref. [13]. The application of these forms to SLs is clearly approximate. We also approximate the phonons in InAs/InGaSb SLs to have the same energy as bulk InAs ones: 30meV. Impact ionization rates are obtained by fitting the Keldysh expression to the microscopic calculations described above. After impact ionization, the initiating carrier is assumed to return to zone center in the lowest energy band. The results of the simulations are analyzed to extract both the carrier distribution functions and drift velocities.

RESULTS

In this section, we present results for two MWIR superlattices (both having 5.7 µm cutoff), 35Å InAs/20Å In$_{0.40}$Ga$_{0.60}$Sb/15Å AlSb and 25Å AlAs/25Å InAs/15Å In$_{0.8}$Ga$_{0.2}$Sb/25Å InAs. In each case, the superlattice unit cell consists of four layers. This adds flexibility to the band engineering in comparison with traditional two-layer superlattices. The superlattices are assumed to be grown on a GaSb substrate and their band structures and impact ionization rates are calculated at 300K.

We present the calculated hole-initiated and electron-initiated impact ionization coefficients for each of these. For hole-initiated impact ionization, the two involved electrons are assumed to be initially in the uppermost spin-split heavy hole band. The initiating hole is permitted to be in the LH$_1$, HH$_1$ or the next highest LH$_2$, HH$_2$ bands. The fourth state, initially unoccupied, is in the lowest or the next lowest conduction bands (C$_1$ or C$_2$). For electron initiated impact ionization, the initiating electron is permitted to be in either the lowest or next lowest two conduction bands (C$_1$, C$_2$ or C$_3$). The other electron is in the HH$_1$, HH$_2$, LH$_1$ or LH$_2$ bands. The third and the forth states, initially unoccupied, are taken to be in the lowest conduction band C$_1$.

A. 35Å InAs/20Å In$_{0.40}$Ga$_{0.60}$Sb/15Å AlSb Superlattice

This superlattice has an energy gap of 220.7 meV at 300K. The net in-plane strain is 0.6 %. The electronic band structure of this superlattice is also designed so that an $E_G = \Delta$ like resonance in the valence band exists, namely the two spin-split LH$_1$ bands are at energy of -240 meV relative to the valence band maximum, approximately equal to the superlattice energy gap.
The LH1 valence band is nearly flat. By contrast, the HH2 valence band is rather dispersive with the HH1-HH2 energy separation 0.1 Å⁻¹ from zone center in the in-plane direction being about 110 meV lower than their 340 meV zone-center energy separation. Also, an $E_G = \Delta$ like resonance in the conduction band is absent. The zone-center energy separation of the C1 and C2 conduction bands of 550 meV is much larger than the energy gap.

The most likely hole-initiated transitions for the same superlattice shows effects similar to those in the SWIR one, namely that the near equality of the zone-center HH1-LH1 separation strongly promotes transitions initiated by holes in LH1. Transitions initiated by holes in HH1 have negligible probability due to the large required momentum transfer, and transitions initiated by holes in the HH2 have a lower probability due to a higher threshold energy.

The most likely electron-initiated transitions plotted for the same superlattice are less probable. Most involve initiating electrons in C2 with very high threshold energy. Transitions with initiating electrons in C1 are possible with a lower threshold but are suppressed by a required large momentum transfer.

Plotted in Fig. 1 is the computed impact ionization rate as function of the initiating electron’s and hole’s energies. For hole-initiated impact ionization, two closely spaced sharp spikes are at energies of –225 meV and –275 meV, and a broader spectrum with a threshold energy at –340 meV are clear. The threshold at –225 meV matches the energy gap. The sharpness of the peaks at –225 meV and –275 meV reflects the flatness of the two spin-split LH1 bands, and the near equality of the zone center HH1-LH1 splitting to the energy gap promotes strong transition amplitudes. The more dispersive HH2 band gives rise to a broad spectrum with a threshold energy of 340 meV, equal to the zone center HH1-HH2 energy separation.

Electron-initiated transitions have a much broader spectrum. Some contributions arise for electrons in C1. Their threshold energy is 340 meV as measured from the bottom of the conduction band, but they are rather weak due to the large required momentum transfer. Initiating electrons in C2 have a high threshold energy of 530 meV but provide a much stronger contribution due to the smaller required momentum transfers.

The low hole threshold energy together with the large impact ionization rate of threshold holes gives rise to a large $\beta$. In contrast, the high threshold energy and weak impact ionization rate for threshold electrons produces a small $\alpha$. The distribution functions for holes and electrons are found to decay exponentially from their respective band edges. Clearly this design fulfills the goal of having its engineered band structure promoting impact ionization by holes through having the energy splitting between the uppermost valence bands being nearly equal to the energy gap. The computed value for $\beta/\alpha$ is 11 for an electric field of 330 kV/cm, using the distribution functions from Monte Carlo solutions to the Boltzmann equation.

B. MWIR 25Å AlAs/25Å InAs/15Å In0.8Ga0.2Sb/25Å InAs Superlattice

This superlattice has an energy gap of 217 meV at 300K. Several features of the band structure are worth noting. The first is the existence of an $E_G = \Delta$ like resonance in the conduction band. Namely, the two spin-split C2 bands are positioned at energy 229 meV above the conduction band minimum, approximately equal to the energy gap (note that zero of the energy scale is the valence band maximum). The second is the nearly dispersionless character of the C2 conduction band, giving rise to a large density of states. The third is the absence of an $E_G = \Delta$ like resonance in the valence band. The LH1 and HH2 valence bands at zone center are positioned at energies of 368 meV and 495 meV below the valence band maximum, respectively.
The most probable electron-initiated transitions demonstrate that the resonance in the conduction band, namely the near equality of the zone-center C1-C2 separation and the energy gap, strongly promotes transitions initiated by electrons in C2. The low threshold energy together with the possibility of transitions with small momentum transfer (and therefore larger transition matrix elements) result in rapid impact ionization rates.

The most likely hole-initiated transitions for the same superlattice are considerably less probable. They involve initiating holes in LH1 with substantially higher threshold energies than the electrons. Thus the band structure of the superlattice appears to fulfill its design goal by providing large electron-initiated impact ionization rates and weak hole initiated ones.

The above qualitative picture is quantitatively verified in Fig. 2. Plotted is the computed impact ionization rate as function of the initiating electrons’ or electron’s energy for the 35Å InAs/20Å In0.40Ga0.60Sb/15Å AlSb superlattice. The threshold energies for various bands and the energy gap of the superlattice are marked.

Figure 1: Computed impact ionization rate as a function of the initiating hole’s or electron’s energy for the 35Å InAs/20Å In0.40Ga0.60Sb/15Å AlSb superlattice. The threshold energies for various bands and the energy gap of the superlattice are marked.

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The above qualitative picture is quantitatively verified in Fig. 2. Plotted is the computed impact ionization rate as function of the initiating electrons’ and holes’ energies. The Monte Carlo methodology for computing the integrals results in some scatter, but general trends are clear. Hole-initiated impact ionization is dominated by two closely spaced sharp spikes that are bound above by energies –495 meV and –368 meV, corresponding to transitions initiated by holes in HH2 and LH1, respectively. Electron initiated impact ionization starts just 229 meV above the conduction band edge, corresponding to a much lower threshold energy than the holes. The near equality of the zone center C1-C2 splitting and the energy gap permits strong transition amplitudes due to near-vertical transitions.
The principal contributions to $\alpha$ arise from non-threshold electrons, ones with energy greater than about 750 meV and are in conduction band C3, for which ionization rates are very large. They rapid impact ionization overwhelms that of threshold holes, resulting in a small $\beta/\alpha$ ratio. The computed value for $\beta/\alpha$ is 0.22 for an electric field of 330 kV/cm, using the distribution functions from Monte Carlo solutions to the Boltzmann equation.

CONCLUSIONS

Sb-based superlattice avalanche photodiodes in the MWIR wavelength range have been examined for potential enhancements of hole-initiated impact ionization rates with the simultaneous suppression of electron-initiated rates, or the reverse. Band engineering of the superlattice band structures produce impact ionization resonances in their valence bands, while preventing similar resonances in the conduction bands, or vice-versa. Fully microscopic calculations have been performed to estimate all parameters that enter into impact ionization coefficients: distribution functions, impact ionization rates, density of states and drift velocities, to estimate $\beta/\alpha$ ratios for two superlattices, both with essentially equal energy gaps in the MWIR. We find that appropriate designs can produce $\beta/\alpha$ ratios either much greater than or much less than 1 at high electric fields. Specifically, $\beta/\alpha$ is larger than one when a relatively high density of states valence band in engineered to be an energy gap below the top of the valence band while simultaneously no conduction band produces a significant enhancement in the conduction band density of states one energy gap above the bottom of the conduction band. On the other hand, $\beta/\alpha$ is smaller than one when a relatively high density of states conduction band in engineered to be an energy gap above the bottom of the conduction band while simultaneously
no valence band produces a significant enhancement in the valence band density of states one energy gap below the top of the valence band. Such band engineering is possible in the type-II Sb-based superlattices in the infrared spectral range. This implies that such superlattices acting as multiplication layers of APDs would provide high gain-bandwidth products and low excess noise factors even under high field conditions. These features predict great promise for superlattice avalanche photodiodes over the full infrared range.

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