Rashba spin-splitting in narrow gap III–V semiconductor quantum wells

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Abstract

Using Kane’s 8-band $k \cdot p$ theory and the envelope function approximation we derive a tight binding Hamiltonian for III–V semiconductor quantum well structures, which accurately models band structure and spin–orbit coupling. By applying a potential difference across the well we have calculated the Rashba spin-splitting in the lowest conduction subband. For identical well widths the Rashba splitting in InSb is shown to be approximately twice that of InAs and, in all cases, passes through a weak maximum with increasing quasimomentum.

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The zero magnetic field spin-splitting ($\delta$) in semiconductor quantum wells (QWs) has been somewhat controversial when the approximate two-band reduced model is used with modified boundary conditions at the heterojunction interfaces [1,2]. This approximation becomes increasingly invalid as the band gap decreases, [3,4] and therefore in this paper, to investigate spin splitting in narrow gap semiconductors (NGS) we use the full 8-band Kane Hamiltonian [5] within the envelope function approximation. The 8-band model was used by de Andrada e Silva et al. [3] to study the Rashba spin-splitting in the CdTe/InSb triangular-well heterojunction and asymmetric square QWS. In this paper we extend this work to narrow InAs and InSb symmetric QWs under an applied bias.

We solve the 8-band Schrödinger equation for III–V semiconductor QWs in the envelope function approximation

$$H \left( k_x, k_y, -i \frac{\partial}{\partial z} \right) f_{k_x, k_y}(z) = E_{k_x, k_y} f_{k_x, k_y}(z),$$

where $f_{k_x, k_y}$ is the 8-component envelope wave function for in-plane quasimomentum $(k_x, k_y)$, and $H$ is the usual $8 \times 8$ matrix differential operator as described, for example, in Ref. [6].

This Hamiltonian depends on the material-dependent band-edge energies at the zone centre for both QW and barriers. However, as shown in Ref. [3] an upper bound on $\delta$ can be obtained by considering barriers with an infinitely wide band gap. In what follows, results are shown for barriers with a conduction and valence band offset of 1 eV, which yields values of $\delta$ to within a few percent of the barrier limit.

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Neglecting the small free-electron kinetic energy term, Eq. (1) reduces to eight first-order differential equations for each \((k_x, k_y)\). These are solved by the finite-difference method with discretisation in the \(z\) direction for which Eq. (1) is equivalent to an eight component tight-binding model. Some care is required when optimising the finite difference mesh to ensure rapid convergence with reducing step-length. For \(N\) finite-difference steps, the resulting \(8N\times8N\) matrix is diagonalised and the spin-split eigenenergies for the lowest conduction subband are extracted. The \(\delta\) for higher subbands rapidly decays to zero.

Calculations were performed for QWs of various widths for both InSb \((E_g = 0.24\ \text{eV}, \ \Delta = 0.81\ \text{eV})\) and InAs \((E_g = 0.41\ \text{eV}, \ \Delta = 0.38\ \text{eV})\). The general behaviour with varying in-plane quasimomentum and potential difference was similar in all cases and we show typical results in Figs. 2 and 3 for wells of width 100 Å with 100 Å wide barriers. The \(\delta\) of the lowest conduction subband as a function of the in-plane quasimomentum in the \(\Gamma \rightarrow X\) direction is plotted for five values of applied bias \((0.05 \rightarrow 0.25\ \text{eV})\).

In Fig. 1 we show that to a good approximation, all values vary linearly with electric field up to the maximum of \(2.5 \times 10^5\ \text{V cm}^{-1}\), consistent with first-order perturbation theory. Here the legend indicates eight different values of \(k_x\) in units of \(10^6\ \text{cm}^{-1}\). We find that \(\delta\) passes through a weak maximum with increasing quasimomentum (Figs. 2 and 3).

The weak maximum is also observed in other \(k\)-space directions and is a consequence of the initial increase of \(\delta\) from zero at the zone centre and an eventual decrease at high energy due to the remoteness of the split-off and heavy-hole bands. The maximum \(\delta\) of InSb QWs is approximately twice that of InAs, due to both the smaller band gap and larger split-off energy of the former, with approximately equally significant contributions from both parameters.

In summary, we have calculated the zero-field spin splittings in an InSb QW, and shown that it is of order twice that of an InAs QW of identical dimensions. Furthermore, the spin-splitting exhibits a weak maximum and remains linear with electric field in the range examined. Future work will take into account electron-electron interactions self-consistently and investigate high field effects.

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Fig. 2. Rashba spin-splitting for a 100 Å InSb quantum well for five different strengths of applied bias.

Fig. 3. Rashba spin-splitting for a 100 Å InAs quantum well for five different strengths of applied bias.

References