Efficient multi-band **k·p** calculations of superlattice electronic and optical properties using plane waves

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***Abstract*—Solving the multi-band k·p Schrödinger equation for a quantum-confined heterostructure using a reciprocal space plane wave approach presents several advantages compared to conventional real space approaches such as the finite difference or element methods. In addition to allowing analytical derivation of the heterostructure Hamiltonian, a desired level of accuracy in the computed eigenstates can generally be achieved using significantly reduced basis set size compared to equivalent real space calculations. This reduces the size of the Hamiltonian matrix that must be diagonalised to compute the electronic structure, thereby accelerating numerical calculations. Here, we demonstrate how the built-in periodicity of plane waves also allows to efficiently compute – for an arbitrary multi-band k·p Hamiltonian – superlattice (SL) miniband structure, using a calculational supercell consisting only of a single SL period. As an example we analyse the origin of the high radiative recombination rate in "broken-gap" InAs/GaSb SLs, of interest for applications in mid-infrared inter-band cascade light-emitting diodes.**

I. Introduction

A combination of accuracy and physical transparency have made multi-band **k·p** calculations the de facto standard approach to compute the optoelectronic properties of quantum-confined heterostructures. Computationally such calculations constitute numerical solution of coupled partial differential equations obtained by quantising the components of the bulk wave vector **k**, with solutions most often employing real space finite difference or element methods to obtain a matrix representation of the Hamiltonian for the calculational supercell. The less commonly employed reciprocal space plane wave expansion method (PWEM) offers advantages including analytical derivation of the supercell Hamiltonian, enhanced numerical efficiency due to the general requirement for smaller basis set size to obtain a given level of accuracy in the computed eigenstates, and removing the requirement to perform numerical quadrature in the computation of matrix elements between eigenstates. Here, we demonstrate that the natural periodicity of plane wave basis states can be exploited to directly and efficiently compute miniband properties in SLs.

The PWEM allows to analyse SL electronic properties using an arbitrary multi-band **k·p** Hamiltonian – including miniband formation and its impact on optical properties – via a calculational supercell consisting of a *single* SL period. As an example we employ an 8-band Hamiltonian to eludicate the nature of radiative recombination in broken-gap (type-III) InAs/GaSb SLs, which are of interest for applications in mid-infrared inter-band cascade light-emitting diodes [1]. Our calculations reveal the important roles played by carrier localisation, as well as miniband occupation and optical selection rules, in determining the radiative recombination coefficient B.

II. Theoretical model

We consider a quantum well (QW) heterostructure in the envelope function approximation, in which the growth axis is aligned with the z-axis of a Cartesian coordinate system. The PWEM consists of writing the Bloch envelope function components as a truncated Fourier series, so that a general eigenstate $|\psi_{n\mathbf{k}}(z)\rangle$ having energy $E_{n\mathbf{k}}$ is given by

$$|\psi_{n\mathbf{k}}(z)\rangle = \sum_{b=1}^{N}\left(\frac{1}{\sqrt{L}}\sum_{m=-M}^{+M} a_{nbm}(\mathbf{k}_{\|},K_z)\,e^{i(G_m+K_z)z}\right)|u_b\rangle\,, \tag{1}$$

where $|u_b\rangle$ are the Bloch basis states of the underlying N-band bulk **k·p** Hamiltonian. The term in parentheses is the expansion of the envelope function $F_{nb\mathbf{k}}(z)$ associated with bulk band b over a supercell of length L, in a periodic basis of plane waves having discrete wave vectors $G_m = \frac{2m\pi}{L}$ [2].

The discrete wave vectors G_m in Eq. (1) describe quantisation along the growth direction z – i.e. that the z component of the wave vector is not a "good" quantum number in a QW. The wave vector $-\frac{\pi}{L} \leq K_z \leq +\frac{\pi}{L}$ describes dispersion associated with the periodicity of the basis states along z, with period L. For a QW calculation it is generally assumed that $K_z = 0$ and dependence on K_z is neglected since (i) thick surrounding barrier layers make L large (K_z small), and (ii) interactions between QW eigenstates from neighbouring supercell periods are an undesirable artefact of the boundary conditions. However, for SL calculations this property can be exploited: if the calculational supercell is set up to contain a single SL period, computing the eigenstates as a function of K_z allows to obtain the electronic properties of an idealised infinite SL. This then allows to explicitly compute the full $\mathbf{k} = (\mathbf{k}_{\|}, K_z)$ dependence of the eigenstates $|\psi_{n\mathbf{k}}(z)\rangle$, which can hence be used directly in conjunction with the supercell Hamiltonian to compute, e.g., optical matrix elements [3], which quantitatively capture the impact of miniband formation.

To obtain energy-dependent (spectral) properties – e.g. density of states, spontaneous emission, etc. – in a conventional QW calculation, it is required to integrate over the in-plane degrees of freedom – i.e. the in-plane wave vector $\mathbf{k}_{\|}$. For a SL this is modified to include miniband dispersion, encapsulating the dependence of the eigenstates on SL wave vector K_z as

$$\int \frac{\mathrm{d}\mathbf{k}_{\|}}{(2\pi)^2} \longrightarrow \left(\frac{2\pi}{L}\right)^{-1}\int_{-\frac{\pi}{L}}^{+\frac{\pi}{L}} \mathrm{d}K_z \int \frac{\mathrm{d}\mathbf{k}_{\|}}{(2\pi)^2}\,, \tag{2}$$

where $\frac{2\pi}{L}$ is the length of the SL Brillouin zone along z.

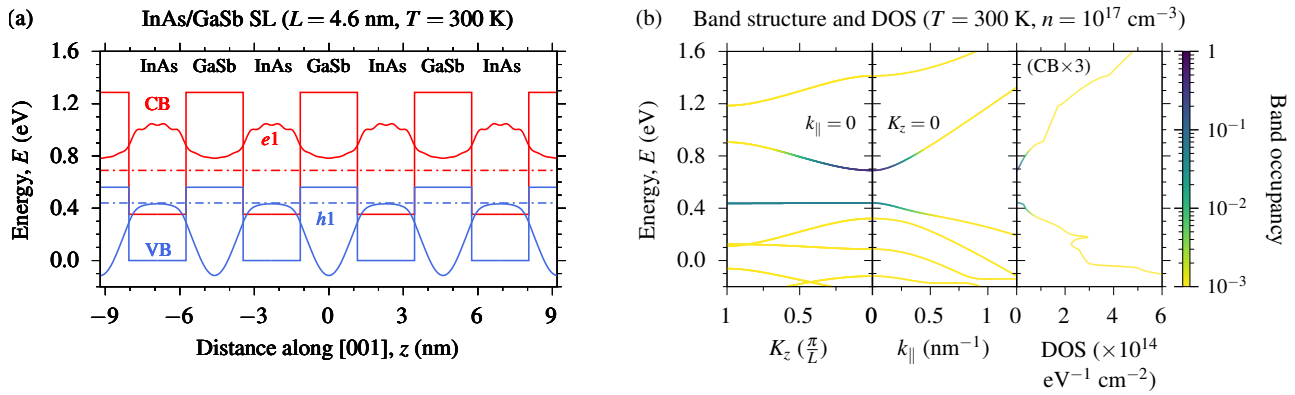

Fig. 1. (a) CB (red) and VB (blue) offsets, and electron (red) and hole (blue) ground state probability densities, for several periods of an InAs/GaSb SL having equal InAs and GaSb layer thickness $t = 2.3$ nm (SL period $L = 4.6$ nm). The dash-dotted red (blue) line shows the calculated electron (hole) ground state energy. (b) SL miniband structure (left-hand panel), in-plane band dispersion (centre panel), and density of states (DOS; right-hand panel) for the InAs/GaSb SL of (a). Line colours in (b) are weighted by Fermi-Dirac electron or hole occupancy, for temperature $T = 300$ K and carrier density $n = 10^{17}$ cm^{-3}.

III. Results

We compute the properties of an InAs/GaSb SL having equal InAs and GaSb layer thickness $t = 2.3$ nm (SL period $L = 2t = 4.6$ nm) using an 8-band **k·p** Hamiltonian. These SLs have recently demonstrated high output power as prototype inter-band cascade light-emitting diodes [1], suggesting high radiative recombination coefficient B. The calculated potential profile and ground state electron ($e1$) and hole ($h1$) probability densities are shown in Fig. 1(a). The SL has type-III band offsets, with the valence band edge of GaSb lying higher in energy than the conduction band edge of InAs. Quantum confinement opens up a band gap, with type-II-like carrier confinement. We find strongly localised holes in GaSb layers, but partially delocalised electrons due to a combination of low InAs electron effective mass and GaSb layer thickness.

Penetration of $e1$ probability density into GaSb layers creates high electron-hole spatial overlap, resulting in inter-band optical matrix elements that are large compared to those expected for spatially indirect transitions. In-plane, the $e1$-$h1$ optical matrix element obeys conventional selection rules, with transverse electric- (TE-) and transverse magnetic-polarised optical transitions being respectively allowed and forbidden at $\mathbf{k}_\parallel = 0$. Our calculations reveal strong K_z dependence of the TE-polarised $e1$-$h1$ optical matrix element – due to combined $e1$ and $h1$ envelope function spatial symmetry, and phase accumulation along K_z – with TE-polarised optical transitions being forbidden at $K_z = \pm\frac{\pi}{L}$. Examining the occupation of electron and hole subbands reveals a strong mismatch in K_z-dependent $e1$ and $h1$ miniband filling (cf. Fig. 1(b)). Since optical transitions require $\Delta\mathbf{k} = 0$, our calculations reveal that mismatch in electron and hole miniband dispersion has the potential to suppress the radiative recombination rate.

To quantify resultant consequences for radiative recombination, we compute the spontaneous emission spectrum which is integrated with respect to photon energy to obtain the radiative current density and hence the radiative recombination coefficient B. Our calculations reveal the complementary and competing effects that govern radiative recombination in these exemplar SLs, and predict quantitatively that InAs/GaSb SLs admit high B values, which we find are comparable with those calculated for novel type-I pseudomorphic [4] and metamorphic [5] QWs having similar (≈ 4 μm) emission wavelengths.

IV. Conclusion

We have demonstrated the ability of the reciprocal space PWEM to efficiently and accurately compute SL optoelectronic properties using an arbitrary multi-band **k·p** Hamiltonian. As an example we analysed radiative recombination in broken-gap InAs/GaSb SLs using an 8-band **k·p** Hamiltonian, where our calculations elucidate and corroborate experimentally observed high optical output power in prototype mid-infrared inter-band cascade light-emitting diodes. These calculations are beyond the capabilities of widely-employed commercial **k·p** software, where SL analysis generally proceeds via "brute force" simulations which require inclusion of many SL periods and do not provide full access to SL miniband dispersion. The PWEM formalism is applicable generally to compute and analyse the properties of SLs whose constituent material band structures can be reliably described using **k·p** theory.

Acknowledgement

This work was supported by the Irish Research Council (Government of Ireland Postgraduate Scholarship GOIPG/2020/1252 to C.M.), by Science Foundation Ireland (project no. 15/IA/3082), and by the National University of Ireland (Post-Doctoral Fellowship in the Sciences to C.A.B.).

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