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ELECTRONIC STRUCTURE CALCULATION OF BULK SEMICONDUCTORS USING THE sp^3s^* EMPIRICAL TIGHT BINDING METHOD

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ABSTRACT

The sp^3s^* empirical tight binding method with fitted input parameters from the literature is used to calculate the band structure of the bulk semiconductor compounds of GaAs and AlAs. Two sets of calculations are performed, namely with and without spin orbit coupling, resulting in 10 and 20 band Hamiltonians, respectively. From these band structures, we then calculate the energy gaps, effective mass of electrons and holes using the curvature method and the corresponding Luttinger parameters. It is found that the energy gaps and effective masses for the spin orbit coupling case are in excellent agreement with their established experimental values. This is as expected as the fitted sp^3s^* input parameters are optimised for the band gaps and effective masses. However, the corresponding Luttinger parameters are poorly estimated by the fitted parameters available in the literature.

INTRODUCTION

Three methods have been widely used for calculating the band structure in bulk semiconductors, namely the tight binding method, the empirical pseudopotential method and the **k.p** perturbation method (Di Carlo 2003). The most economical approach for energy band computations in semiconductors is the envelope function approximation or multiband **k.p** method. It uses a minimal set of parameters that are determined empirically from experiments. By means of a perturbative approach, it provides a continuation in the wave vector $\boldsymbol{k}$ of the energy bands in the vicinity of some special points in the Brillouin zone. In the tight binding approach introduced by Slater & Koster (1954), the electronic states are considered to be linear combinations of atomic (*s,p,d,…*) orbitals, and thus it is also known as the Linear Combination of Atomic Orbital (LCAO) method. Here, the Hamiltonian matrix elements between the atomic orbital states are not evaluated directly, but are instead introduced as free parameters. In the more sophisticated but computer-intensive empirical pseudopotential model, the crystal potential is represented by a linear superposition of atomic potentials, which are modified to obtain good fits to the experimental direct and indirect band gaps and effective masses (Vurgaftman *et al.* 2001).

In this paper, we apply the nearest neighbour sp^3s^* empirical tight binding method in the calculation of the band structure, effective mass and Luttinger parameters for bulk semiconductor materials. Our main objective is to assess the quality and suitability of

the available fitted parameters for this method in future modelling of the electronic properties of such semiconductor materials and their heterostructures. Various flavours of the tight binding method exist and different sets of input parameters have been fitted for their empirical versions covering a wide range of atoms, atomic orbitals, nearest neighbours and spin orbit consideration (Slater & Koster 1954, Chadi 1997, Vogl *et al.* 1983, Boykin 1997, and Jancu *et al.* 2002). We have previously performed certain aspects of the electronic structure calculation using the nearest neighbour sp^3s^* tight binding method without spin orbit coupling to test its validity for silicon, GaAs and AlAs (Zulkifli *et al.* 2004).

THEORY

In a crystalline bulk material, the symmetry of the system reduces the problem to the primitive unit cell; and its one-electron wave functions, $|n\mathbf{k}\rangle$, can be written as Bloch waves (Di Carlo 2003) ,

$$\left|n\vec{k}\right\rangle = \sum_{\alpha\beta} C_{\alpha,\beta}\left(n,\vec{k}\right)\left\{\sum_{R} e^{i\vec{k}.\vec{R}_\beta}\left|\alpha,\vec{R}_\beta\right\rangle\right\}. \tag{1}$$

Here we conveniently write $\vec{R}_\beta = \vec{R} + \vec{V}_\beta$, where **R** is the lattice vector; **v** is the base atom displacement and the subscripts β and α refer to the base atom index and to the atomic orbital index, respectively. The parameters $C_{\alpha\beta}\left(n,\vec{k}\right)$ are the coefficients of the linear combination that are dependent on the band index n and on the wave vector $\boldsymbol{k}$. For a bulk semiconductor with zinc blende symmetry, the sp^3s^* tight-binding model without spin-orbit interaction introduced by Vogl *et al.* (1983) uses one s state and three p states plus an excited state of s^* for a basis atom, resulting in 10 orbitals for a primitive cell that contains two atoms. This method needs 13 fitted input parameters that were determined by comparison with experimental data. These interaction parameters are basically independent matrix elements, comprising of six on-site energies of ε_{sa} , ε_{sc} , ε_{pa} , ε_{pc} , ε_{s*a} and ε_{s*c} ; with $\alpha = a$ (anion) , c (cation); and seven hopping terms of $V_{ss} = 4t_{ss}\left(\vec{R}_a - \vec{R}_c\right)$; $V_{xy} = 4t_{p_x p_y}\left(\vec{R}_a - \vec{R}_c\right)$; $V_{ps} = 4t_{p_x s}\left(\vec{R}_a - \vec{R}_c\right)$; $V_{ps*} = 4t_{p_x s*}\left(\vec{R}_a - \vec{R}_c\right)$; $V_{xx} = 4t_{p_x p_x}\left(\vec{R}_a - \vec{R}_c\right)$; $V_{sp} = 4t_{sp_x}\left(\vec{R}_a - \vec{R}_c\right)$ and $V_{s*p} = 4t_{s*p_x}\left(\vec{R}_a - \vec{R}_c\right)$.

For a zinc blende crystal of lattice constant a, the k dependence in this tight binding picture is given by defining the g_i coefficients,

$$g_0(k) = \frac{1}{4}\left[e^{i\vec{k}\cdot\vec{\tau}_1} + e^{i\vec{k}\cdot\vec{\tau}_2} + e^{i\vec{k}\cdot\vec{\tau}_3} + e^{i\vec{k}\cdot\vec{\tau}_4}\right];\; g_1(k) = \frac{1}{4}\left[e^{i\vec{k}\cdot\vec{\tau}_1} - e^{i\vec{k}\cdot\vec{\tau}_2} + e^{i\vec{k}\cdot\vec{\tau}_3} - e^{i\vec{k}\cdot\vec{\tau}_4}\right]$$

$$g_2(k) = \frac{1}{4}\left[e^{i\vec{k}\cdot\vec{\tau}_1} - e^{i\vec{k}\cdot\vec{\tau}_2} - e^{i\vec{k}\cdot\vec{\tau}_3} + e^{i\vec{k}\cdot\vec{\tau}_4}\right];\; g_3(k) = \frac{1}{4}\left[e^{i\vec{k}\cdot\vec{\tau}_1} + e^{i\vec{k}\cdot\vec{\tau}_2} - e^{i\vec{k}\cdot\vec{\tau}_3} - e^{i\vec{k}\cdot\vec{\tau}_4}\right] \tag{3}$$

where the vectors τ_i point to the nearest neighbour atoms and are given by $\vec{\tau}_1 = \frac{a}{4}[1,1,1]$; $\vec{\tau}_2 = \frac{a}{4}[-1,-1,1]$; $\vec{\tau}_3 = \frac{a}{4}[1,-1,-1]$ and $\vec{\tau}_4 = \frac{a}{4}[-1,1,-1]$.

Thus, the sp^3s^* model without spin orbit coupling applied to a zinc blende crystal results in a 10x10 Hamiltonian,

$$\begin{bmatrix}
E_{sa} & 0 & 0 & 0 & 0 & V_{ss}g_0 & V_{sp}g_1 & V_{sp}g_2 & V_{sp}g_3 & 0 \\
0 & E_{pa} & 0 & 0 & 0 & -V_{ps}g_1 & V_{xx}g_0 & V_{xy}g_3 & V_{xy}g_2 & V_{ps*}g_1 \\
0 & 0 & E_{pa} & 0 & 0 & -V_{ps}g_2 & V_{xy}g_3 & V_{xx}g_0 & V_{xy}g_1 & V_{ps*}g_3 \\
0 & 0 & 0 & E_{pa} & 0 & -V_{ps}g_3 & V_{xy}g_2 & V_{xy}g_1 & V_{xx}g_0 & V_{ps*}g_3 \\
0 & 0 & 0 & 0 & E_{s*a} & 0 & V_{s*p}g_1 & V_{s*p}g_2 & V_{s*p}g_3 & 0 \\
V_{ss}g_0^* & -V_{ps}g_1^* & -V_{ps}g_2^* & -V_{ps}g_3^* & 0 & E_{sc} & 0 & 0 & 0 & 0 \\
V_{sp}g_1^* & V_{xx}g_0^* & V_{xy}g_3^* & V_{xy}g_2^* & V_{s*p}g_1^* & 0 & E_{pc} & 0 & 0 & 0 \\
V_{sp}g_2^* & V_{xy}g_3^* & V_{xx}g_0^* & V_{xy}g_1^* & V_{s*p}g_2^* & 0 & 0 & E_{pc} & 0 & 0 \\
V_{sp}g_3^* & V_{xy}g_2^* & V_{xy}g_1^* & V_{xx}g_0^* & V_{s*p}g_3^* & 0 & 0 & 0 & E_{pc} & 0 \\
0 & V_{ps*}g_1^* & V_{ps*}g_3^* & V_{ps*}g_3^* & 0 & 0 & 0 & 0 & 0 & E_{s*c}
\end{bmatrix} \quad (2)$$

The interaction of spin and orbit, also known as spin orbit coupling, was added to the empirical tight binding model by Chadi (1977). For a spherically symmetric potential, the spin orbit interaction is given by

$$\vec{H}_{SO} = \frac{\hbar}{4m^2c^2}\frac{1}{r}\frac{dV_c(\vec{r})}{dr}\vec{L}\cdot\vec{\sigma} \quad (4)$$

where σ are the Pauli matrices, V_c is the crystal potential and **L** is the angular momentum. By explicitly considering the spin index σ = ↑,↓ in the localised basis, the spin orbit matrix elements become

$$\left\langle \alpha,\vec{R}_\beta,\sigma\middle|\vec{H}_{SO}\middle|\alpha',\vec{R}_\beta,\sigma'\right\rangle = \left\langle \alpha\vec{R}_\beta\middle|\frac{\hbar}{2m^2c^2}\frac{1}{r}\frac{dV_c(r)}{dr}\vec{L}\middle|\alpha'\vec{R}'_{\beta'}\right\rangle\cdot\left\langle\sigma\middle|\vec{\sigma}\middle|\sigma'\right\rangle. \quad (5)$$

If we consider only contributions on the same atom, then the only non-zero matrix elements are

$$\begin{gathered}
\left\langle p_x,\vec{R}_\beta,\uparrow\middle|H_{SO}\middle|p_y,\vec{R}_\beta,\uparrow\right\rangle = -i\lambda_\beta;\left\langle p_x,\vec{R}_\beta,\downarrow\middle|H_{SO}\middle|p_y,\vec{R}_\beta,\downarrow\right\rangle = i\lambda_\beta \\
\left\langle p_z,\vec{R}_\beta,\uparrow\middle|H_{SO}\middle|p_x,\vec{R}_\beta,\downarrow\right\rangle = -\lambda_\beta;\left\langle p_x,\vec{R}_\beta,\downarrow\middle|H_{SO}\middle|p_y,\vec{R}_\beta,\uparrow\right\rangle = \lambda_\beta \quad (6) \\
\left\langle p_y,\vec{R}_\beta,\uparrow\middle|H_{SO}\middle|p_z,\vec{R}_\beta,\downarrow\right\rangle = -i\lambda_\beta;\left\langle p_y,\vec{R}_\beta,\downarrow\middle|H_{SO}\middle|p_z,\vec{R}_\beta,\uparrow\right\rangle = -i\lambda_\beta
\end{gathered}$$

and their complex conjugates. Here $\lambda_\beta = \lambda_a$, λ_c are the spin orbit splitting of the anion and cation p states, which in the empirical tight binding philosophy are fitting parameters. The inclusion of the spin orbit interaction in the sp^3s^* tight binding model yields, for a zinc blende structure, a 20x20 Hamiltonian matrix which must be diagonalised for each $\boldsymbol{k}$ vector to obtain the bulk band structure and other electronic properties.

The effective mass of a semiconductor is obtained by fitting the actual E-k diagram around the conduction band minimum or the valence band maximum by a parabola. Most semiconductors can be described as having one band minimum at k=0 as well as several equivalent anisotropic band minima at $k \neq 0$. In addition, there are three band maxima of interest that are close to the valence band edge (Van Zeghbroeck 2004). To fit the effective mass we must analytically diagonalise the Hamiltonian in the neighbourhood of Γ and differentiate twice with respect to $\boldsymbol{k}$ to get the curvature. Effective mass is defined by analogy with Newton's second law, $\mathbf{F}=m\mathbf{a}$. From the external electric field alone of $\mathbf{E}$, the electron would experience a force of $q\mathbf{E}$, where q is the charge. Hence under the model that only an external electric field acts, the effective mass m^* is just proportional to the inverse curvature of a parabolic band (Aschroft & Mermin 1981; Kittel 1996),

$$m^* = \hbar^2 \cdot \left[\frac{d^2E}{dk^2}\right]^{-1} \quad . \tag{7}$$

In practice, we solve equation (7) by approximating the derivative by finite differences,

$$\left.\frac{d^2E}{dk^2}\right|_i \approx \frac{E_{i-1} - 2E_i + E_{i+1}}{(\Delta k)^2} . \tag{8}$$

For a free particle, the dispersion relation is a quadratic, and so the effective mass would be constant, and equal to the real mass. In a crystal, the situation is far more complex. The dispersion relation is not even approximately quadratic, in the large scale. However, wherever a minimum occurs in the dispersion relation, the minimum can be approximated by a quadratic curve in the small region around that minimum. Hence, for electrons having energies close to a minimum, effective mass is a useful concept.

In the effective mass or **k.p** perturbative theory, the acceptor binding energy depends on the three Luttinger parameters of γ_1 , γ_2 and γ_3. These, in turn, can be related to the heavy-hole (HH), light-hole (LH) and spin orbit split-off (SO) masses along the ΓX=(100), ΓK=(110) and ΓL=(111) symmetry axes by (Vurgaftman *et al.* 2001):

$$\frac{1}{m_{HH}^X} = \gamma_1 - 2\gamma_2 \quad ; \quad \frac{1}{m_{HH}^K} = \frac{1}{2}(2\gamma_1 - \gamma_2 - 3\gamma_3) \quad ; \quad \frac{1}{m_{HH}^L} = \gamma_1 - 2\gamma_3$$

$$\frac{1}{m_{LH}^X} = \gamma_1 + 2\gamma_2 \quad ; \quad \frac{1}{m_{LH}^K} = \frac{1}{2}(2\gamma_1 + \gamma_2 + 3\gamma_3) \quad ; \quad \frac{1}{m_{LH}^L} = \gamma_1 + 2\gamma_3 \tag{9}$$

$$\frac{1}{m_{SO}^X} = \gamma_1 - \frac{E_P\Delta_o}{3E_g^\Gamma\left(E_g^\Gamma + \Delta_o\right)} .$$

The various effective masses in these expressions and throughout this work are given in units of the free electron mass. Here, E_g^Γ is the Brillouin zone centre band gap, Δ_o is the

spin orbit splitting (i.e. the splitting of the top most valence band at the Brillouin zone centre of Γ) and E_P is an interaction energy. By rearranging the equations, we arrive at four equivalent expressions for γ_1,

$$\gamma_1^X = \frac{1}{2}\left[\frac{1}{m_{LH}^X} + \frac{1}{m_{HH}^X}\right]; \quad \gamma_1^K = \frac{1}{2}\left[\frac{1}{m_{LH}^K} + \frac{1}{m_{HH}^K}\right]; \quad \gamma_1^L = \frac{1}{2}\left[\frac{1}{m_{LH}^L} + \frac{1}{m_{HH}^L}\right];$$

$$\gamma_1^{SO} = \frac{1}{2}\left[\frac{1}{m_{SO}^X} + \frac{E_p \Delta_O}{3E_g^\Gamma \left(E_g^\Gamma + \Delta_O\right)}\right] \quad (10)$$

and respectively unique expressions for γ_2 and γ_3,

$$\gamma_2 = \frac{1}{4}\left[\frac{1}{m_{LH}^X} - \frac{1}{m_{HH}^X}\right]; \qquad \gamma_3 = \frac{1}{4}\left[\frac{1}{m_{LH}^L} - \frac{1}{m_{HH}^L}\right]. \quad (11)$$

Thus, knowing the effective masses from the tight binding calculations enables us to estimate the Luttinger parameters that are used as inputs for the **k.p** approach of electronic structure calculation. The fact that the Luttinger parameters depend on the valence band masses in the *ΓX*, *ΓK* and *ΓL* directions suggests that the band gaps and the effective masses need to be fitted properly in the tight binding parametrisation scheme. In the "empirical" tight binding approach, these input or interacting parameters are fitted from the experimental values of the band gaps and effective masses.

Table 1: Input parameters for the sp^3s^* tight binding calculation, with SO for the spin orbit coupling case. These fitted values are taken from [a]Boykin et al. (1997) and [b]Menchero and Boykin (1999).

Parameter	GaAs[b]	GaAs (SO)[a]	AlAs[a]	AlAs (SO)[a]
E_{sa}	-8.48706	-8.510704	-8.26631	-8.38116
E_{pa}	0.38769	0.954046	6.34429	0.22944
E_{sc}	-2.86111	-2.774754	-1.78202	1.74467
E_{pc}	3.56769	3.434046	2.94769	2.83284
E_{s*a}	8.48769	8.454046	6.845424	6.730574
E_{s*c}	6.61769	6.584046	6.08769	5.97284
V_{ss}	-6.56053	-6.45130	-6.6642	-6.6642
V_{xx}	2.26095	1.9546	1.878	1.8780
V_{xy}	5.6000	4.7700	3.8600	3.8600
V_{sp}	4.6800	4.6800	5.6000	5.6000
V_{ps}	8.000	7.700	7.6000	6.8000
V_{s*p}	4.6500	4.8500	4.22	4.2200
V_{ps*}	6.000	7.0100	8.3000	7.3000
λ_a	0	0.14	0	0.14
λ_c	0	0.058	0	0.008

As listed in Table 1, our sp^3s^* tight binding calculations adopt the fitted parameters of Boykin *et al.* (1997) and Menchero and Boykin (1999) for the bulk semiconductor compounds of GaAs and AlAs. We also use the values of E_P as 28.8 eV for GaAs and 21.1 eV for AlAs (Vurgaftman *et al.* 2001).

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RESULT AND DISCUSSION

We have applied the sp^3s^* empirical tight binding method to the band structure calculation for the two bulk semiconductor compounds of GaAs and AlAs. The calculations are performed for the cases of with and without spin orbit couplings. The band structure along the symmetry axes of *ΓKLΓXU* for the bulk compounds of GaAs and AlAs are given in Figures 1 and 2, respectively. Here, $\Gamma=(0,0,0)2\pi/a$ is the Brillouin zone centre; and $X=(1,0,0)2\pi/a$, $L=(½,½,½)2\pi/a$, $K=(0,¾,¾)\ 2\pi/a$ and $U=(1,½,½)\ 2\pi/a$ are the Brillouin zone edges for a zinc blende crystal of lattice constant *a*. We use a = 6.53Å for GaAs and a = 6.56Å for AlAs (Vurgaftman *et al.* 2001). Spin orbit couplings need to be included in the calculations as the corresponding splittings, Δ_o, in the materials of 0.36 eV for GaAs and 0.34 eV for AlAs are significant compared to their respective band gaps.

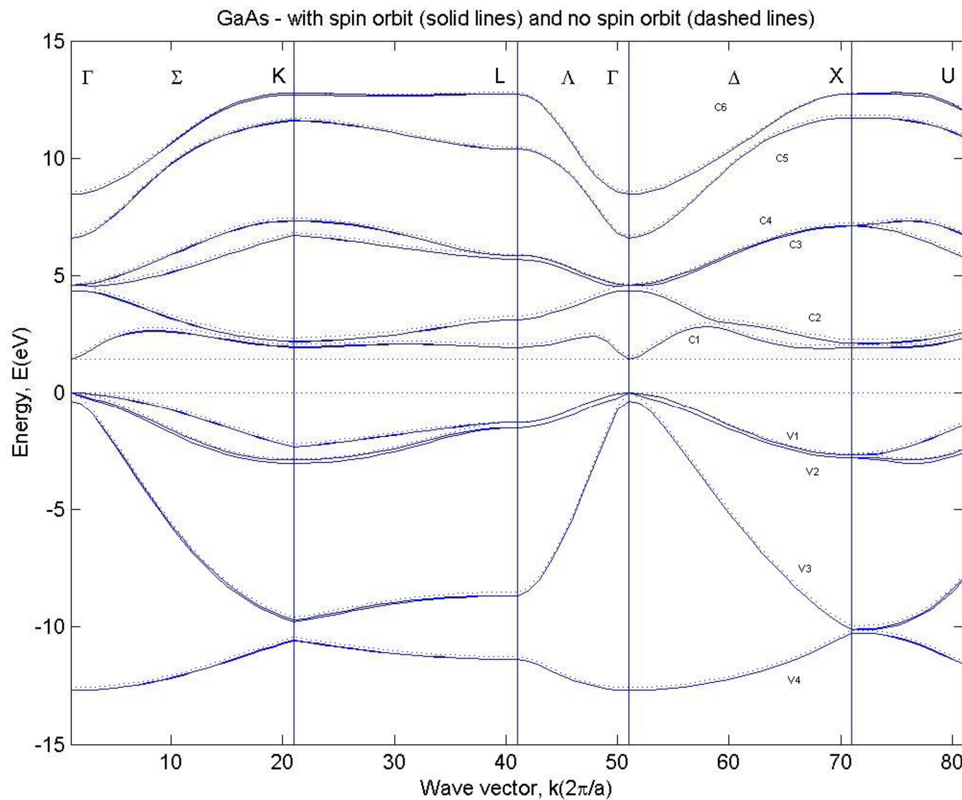

Figure 1: Calculated sp^3s^* band structure of bulk GaAs.

Shown in Figure 1 are the dispersion curves, or $E=E(k)$, for ten bulk bands of GaAs for sp^3s^*, comprising the four highest valence bands of V1-V4 and the six lowest conduction bands of C1-C6. These band structures exhibit certain features that are common to bulk semiconductors. There are fundamental differences between the band structures. It is seen from the figure and Table 2 that GaAs is a direct gap semiconductor with a minimum band gap of E^{Γ}_g=1.54 eV in the absence of spin orbit

coupling; which decreases to 1.42 eV when spin orbit interaction is included. It is also observed that the bands are spin-degenerate only along *LΓX*; along other axes the bands could spin-split.

Figure 2 shows that AlAs is an indirect gap material with a minimum gap along *X* of $E^X{}_g$= 2.29 eV for no spin orbit interaction and 2.28 eV with spin orbit interaction. It has an extremum gap at *Γ* of $E^\Gamma{}_g$ = 3.03 eV for no spin orbit interaction and 3.02 eV for spin orbit interaction. Table 3 summarises the calculated energy gaps for AlAs.

Table 2: Calculated sp^3s* electronic structure parameters for GaAs. All established values are taken from Vurgaftman *et al.* (2001); except [a]Loehr *et al.* (1997); [b]Boykin *et al.* (1999); [c]Menchero & Boykin (1999).

Parameters	No spin orbit	With spin orbit	Established Values
$E_g^\Gamma(eV)$	1.538	1.417	1.42(300K), 1.52(0K), 1.424[d]
$E_g^X(eV)$	2.049	1.927	1.981
$E_g^K(eV)$	2.072	1.936	-
$E_g^L(eV)$	1.889	1.77	1.815
Δ_0	-	0.364	0.341, 0.37[b]
$m_e^\Gamma(C1)$	0.069	0.068	0.067, 0.068[b], 0.067[d]
$m_{HH}^\Gamma(V1)$	0.466(X),0.885(L), 1.605(K)	0.446(X),0.877(L), 0.714(K)	0.45(X), 0.35(X)[a], 0.41(X)[b], 0.44(X)[c],0.874(K)[c] 0.45(X)[d]
$m_{LH}^\Gamma(V2)$	0.466(X),0.885(L), 0.466(K)	0.070(X),0.065(L), 0.066(K)	0.08(X), 0.071(X)[b], 0.07(X)[c], 0.065(K)[c], 0.082(X)[d]
$m_{so}^\Gamma(V3)$	0.053(X),0.048(L), 0.049(K)	0.145	0.172, 0.14[b]

Table 3: Calculated sp^3s* electronic structure parameters for AlAs. All established values are taken from Vurgaftman *et al.* (2001); except [a]Loehr *et al.* (1997), [c]Menchero & Boykin (1999), and [d]Singh (1999).

Parameters	No spin orbit	With spin orbit	Established values
$E_g^\Gamma(eV)$	3.026	3.025	3.099, 2.153[d]
$E_g^X(eV)$	2.289	2.277	2.24
$E_g^K(eV)$	2.722	2.703	-
$E_g^L(eV)$	2.766	2.761	2.46
Δ_0	-	0.337	0.28
$m_e^\Gamma(C1)$	0.141	0.182	0.15, 0.1[d]
$m_{HH}^\Gamma(V1)$	0.764(X),1.385(L), 2.334(K)	0.747(X),1.363(L), 1.142(K)	0.42(X)[a], 0.745(X)[c], 1.371(K)[c]
$m_{LH}^\Gamma(V2)$	0.764(X),1.385(L), 0.764(K)	0.135(X),0.125(L), 0.127(K)	0.136(X)[c], 0.126(K)[c]
$m_{so}^\Gamma(V3)$	0.079(X),0.072(L), 0.073(K)	0.247(L)	0.28

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From these band structures, we have computed the effective masses for the lowest electron, heavy hole, light hole and spin orbit split-off along the *ΓX, ΓK* and *ΓL* directions; for both with and without spin orbit coupling. So, there are eight independent masses along each direction, with four for the band structure without spin orbit coupling of $m_{C1}^{\Gamma}, m_{V1}^{\Gamma}, m_{V2}^{\Gamma}$ and m_{V3}^{Γ}; and the other four of $m_{e}^{\Gamma}, m_{HH}^{\Gamma}, m_{LH}^{\Gamma}$ and m_{SO}^{Γ} are for the band structure with spin orbit coupling. Tables 2 and 3 show our results using the curvature method from the band structure for the GaAs and AlAs compounds. For comparison we have included their established experimental values found in the literature. Our calculated effective mass values in both of these compound semiconductors for the lowest electrons are in very good agreement with the recommended values. This is to be expected as the input parameters that we used were optimally fitted for the effective masses (Boykin *et al.* 1997). The effective masses of the split-off bands with spin orbit interaction are also in good agreement with the established values. This is due to the electron-like nature of the split-off band. However, the calculated effective masses for the heavy and light holes do not agree well with their established values, even under spin orbit coupling. Furthermore, there are wide discrepancies in their established or experimental values due to measurement difficulties. It is also observed that with spin orbit coupling, in both compounds the lowest electrons and split off bands are perfectly isotropic, the light holes are almost isotropic, whereas the heavy holes are very anisotropic.

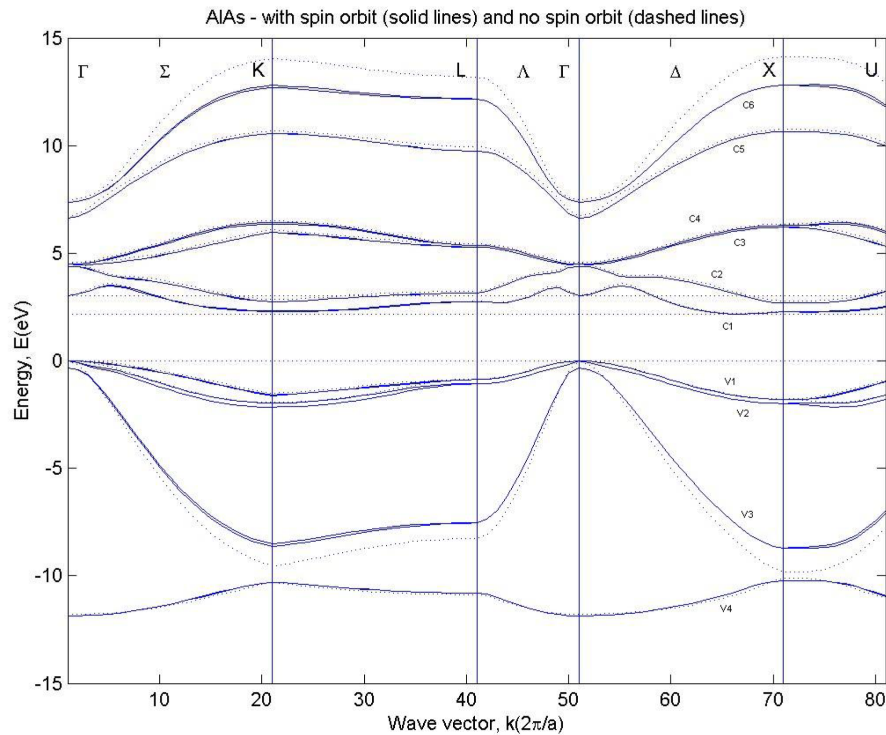

Figure 2: Calculated sp^3s^* band structure of bulk AlAs.

Table 4 presents the calculated Luttinger parameters from our tight binding model. There is reasonable agreement and consistency among the different expressions for γ_1 for both the compounds. However, comparing all the calculated Luttinger parameter values with their corresponding established values (Vurgaftman *et al.* 2001) shows that the two sets are significantly different for both the bulk compounds of GaAs and AlAs. Thus, the fitted parameters in the literature for the sp^3s^* model that we use (Boykin *et al*. 1997 and Menchero and Boykin 1999) fail to satisfactorily reproduce the set of Luttinger parameter values. This limits the usefulness of the output of the present calculation in further electronic structure modelling, such as in **k.p** theory. So, for applications that require the use of Luttinger parameters, a suitably fitted set of tight binding parameters should be used.

Table 4: Calculated Luttinger parameters, γ_i, using sp^3s^* with spin orbit coupling for GaAs and AlAs. For comparison, the established experimental values (Exp.) from Vurgaftman *et al.* (2001) are also shown.

γ_i	GaAs		AlAs	
	Calculated	Exp.	Calculated	Exp.
γ_1	8.264(X), 8.276(K), 8.263(L), 8.859(SO)	6.98	4.373(X), 4.375(K), 4.367(L), 4.757(SO)	3.76
γ_2	3.011	2.06	1.519	0.82
γ_3	3.561	2.93	1.817	1.42

CONCLUSION

We have used the available fitted parameters for the sp^3s^* empirical tight binding method to calculate the electronic structure of the popular bulk semiconductor compounds of GaAs and AlAs with crystal lattices of zinc blende symmetry. We have calculated the band structures, effective masses using the curvature method and the related set of Luttinger parameters for these materials. We found that the fitted parameters predicted well the energy gaps and certain effective masses but the calculated Luttinger parameters are significantly different from their established values. This arises from the band gap and effective mass optimisation of the fitted input parameters for this particular tight binding procedure. Thus, we should use these input parameters with caution in future calculation and modelling of the various electronic, optical and transport properties of bulk semiconductors and their heterostructures.

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