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PROMIS

PROMIS – Postgraduate Research on Dilute Metamorphic Nanostructures and Metamaterials in Semiconductor Photonics

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D1.2 Band structure parameters established for relevant III-V(N) heterostructures

1. Introduction

The PROMIS consortium is interested in a range of different dilute nitride III-V semiconductor alloys. Theoretical modelling is being used to provide relevant band structure information to support the design, development and analysis of dilute nitride metamorphic nanostructures across the PROMIS consortium. Tight-binding (TB) calculations have been undertaken to establish the impact of N on the electronic structure of GaSbN and InGaAsN layers grown on GaAs (WP1, WP3) and of InAsSbN grown on InAs/AlAsSb (WP4). The results of these models are being used as input to **k.p** models to:

- support the design and analysis of single photon sources in collaboration with ROME & UMR (WP1),
- optimise the electronic and optical properties of GaSbN QDs for CPV solar cells grown by ULANC (WP3)
- design and optimise the emission characteristics of Type-II InAsSbN/InAs/AlAsSb structures grown by ULANC for mid-IR LED applications (WP4).

This work requires appropriate TB and **k.p** band structure parameters to describe the following binary materials alloyed with N:

- GaAs
- InAs
- GaSb
- InSb

We first present below in section 2 the tight-binding parameters that we have developed for these materials, and then present in section 3 **k.p** parameters derived from the TB band structure analysis.

2. Tight-binding parameters for III-V(N) materials

Previous work at Tyndall has shown that the effect of N on the band structure of III-V(N) alloys can be well described using an sp^3s^* tight-binding Hamiltonian. TB band structure parameters have been derived and presented for GaSb and InSb in [1] and for GaAs and InAs in [2]. The GaAs and InAs parameters were subsequently updated to provide improved description of isolated N and N pair states. The GaSb and InSb parameters from [1] and the updated III-As parameters [3] are reproduced in Table 1 below.

3. k.p parameters for III-V(N) materials

We use a ten-band **k.p** Hamiltonian [4] to describe the electronic structure of the III-V(N) nanostructures. This Hamiltonian includes the doubly degenerate heavy-hole (HH), light-hole (LH) and spin-split-off (SO) valence bands and the lowest conduction (CB) bands included in a conventional eight-band Hamiltonian. It also includes a pair of doubly degenerate N resonant defect bands which lie close in energy to the CB states, with which they have a strong band-anticrossing interaction.

Suitable 8-band **k.p** parameters are well established for conventional III-V semiconductors and for conventional alloys such as $In_{1-x}Ga_xAs$. We take the 8-band **k.p** parameters for GaSb and InSb from

Vurgaftman *et al.* [5]. The choice of material parameters used to model InGaAs alloys is described in Ref. [3]. All material parameters for this alloy are interpolated linearly from those of the constituent binary compounds, except for the band gap and spin-orbit-splitting energy, which include bowing terms and are calculated according to Ref. [6]. The temperature dependence of the band gaps of the constituent binary compounds are calculated using the Varshni relation [5]. The 8-band **k.p** band parameters for GaAs, InAs, GaSb and InSb are presented in Table 2.

It is well-established that when a single N atom replaces an As atom in GaAs, it forms a resonant defect level above the CBE of GaAs [7]. This defect level arises because of the large difference in electronegativity and atomic size between N and As [8,9]. The BAC model introduced by Walukiewicz and co-workers explains the extreme band gap bowing observed in $Ga_{1-y}In_yN_xAs_{1-x}$ in terms of an interaction between two levels, one at energy E_N associated with these localized N impurity states ψ_N, and the other at energy E_c associated with the extended CBE state ψ_{c0} of the GaInAs matrix, with the two states linked by a matrix element V_{Nc} describing the interaction between them [10]. The conduction band dispersion of $GaInN_xAs_{1-x}$ is then given in the BAC model by the lower eigenvalue of the determinant

$$\begin{vmatrix} E_N & V_{Nc} \\ V_{Nc} & E_c + \frac{\hbar^2 k^2}{2m_c^*} \end{vmatrix} \qquad (1)$$

where m^*_c is an appropriately chosen band edge effective mass for the Ga(In)As host matrix material [11]. Since the interaction V_{Nc} is between a localised N state and the extended host matrix CBE, V_{Nc} therefore increases with N composition x as $x^{½}$ [12], and is generally given by

$$V_{Nc} = \beta\, x^{½} \qquad (2)$$

We have used the sp^3s^* TB Hamiltonian to calculate the energy of the isolated N state, E_N, for the four binary XY compounds with X = Ga, In, and Y = As, Sb. We can also extract from the calculations the magnitude of the interaction parameter β linking the isolated N states and the conduction band edge. Table 3 lists the calculated values of E_N and β as well as the band gap energy for the six binary compounds considered. These N-related parameters can then be combined with the 8-band **k.p** parameters in Table 2 to give the 10-band **k.p** Hamiltonian for the dilute nitride alloys under investigation in PROMIS.

Parameter	GaAs	InAs	GaN	InN	GaSb	InSb
a(Å)	5.6532	6.0583	4.4900	4.9850	6.0959	6.4794
ΔE_V (eV)	0.00	0.21	-2.28	-2.00	0.67	0.83
$E_{s_a^*}$ (eV)	7.0914	7.2730	12.2000	12.2000	6.6354	6.4530
$E_{s_c^*}$ (eV)	6.2000	6.6095	12.2000	12.2000	5.9846	5.9362
E_{s_a} (eV)	−8.6336	−9.5381	−12.3306	−12.8406	−7.3207	−8.0157
E_{s_c} (eV)	−2.9474	−2.7219	−0.9994	−0.3794	−3.8993	−3.4643
E_{p_a} (eV)	0.9252	0.7733	2.7120	2.2260	0.8554	0.6738
E_{p_c} (eV)	3.5523	3.5834	8.5803	8.2718	2.9146	2.9162
Δ_a (eV)	0.4050	0.3870	0.0210	0.0060	0	0
Δ_c (eV)	0.1650	0.4155	0.0060	0.0030	0	0
$V_{ss\sigma}$ (eV)	−1.6835	−1.4013	−2.0700	−1.5501	−1.5392	−1.3798
$V_{s_a^* p_c \sigma}$ (eV)	2.0400	1.3939	1.5442	0.4898	2.1605	1.5444
$V_{s_c^* p_a \sigma}$ (eV)	1.7700	1.6123	2.8375	2.3295	1.8264	1.4743
$V_{s_a p_c \sigma}$ (eV)	2.3920	1.3079	2.0717	0.7974	2.1478	1.6403
$V_{s_c p_a \sigma}$ (eV)	2.4200	2.3337	3.0593	2.5956	2.0211	1.9875
$V_{pp\sigma}$ (eV)	2.9500	2.6588	5.0530	4.5382	2.4590	2.2885
$V_{pp\pi}$ (eV)	−0.7420	−0.6390	−0.7150	−0.6592	−0.6374	−0.6186
$\eta_{ss\sigma}$	3.512	3.512	2.910	2.810	3.66	3.66
$\eta_{s_a^* p_c \sigma}$	4.200	4.200	4.000	3.000	4.20	4.20
$\eta_{s_c^* p_a \sigma}$	7.200	7.200	6.200	6.200	7.20	7.20
$\eta_{s_a p_c \sigma}$	4.100	4.100	3.000	3.000	4.08	4.08
$\eta_{s_c p_a \sigma}$	4.500	4.500	4.580	4.580	4.09	4.09
$\eta_{pp\sigma}$	3.204	3.204	2.091	2.091	2.20	2.20
$\eta_{pp\pi}$	4.236	4.236	3.724	3.724	3.24	3.24

Table 1: Material parameters for zinc blende III-V compounds used in sp^3s^* tight-binding calculations.

Parameter	GaAs	InAs	GaSb	IuSb	GaN	InN
$Eg\ (eV)$	1.519	0.418	0.812	0.235		
	(1.422)	(0.355)	(0.727)	(0.174)		
$\Delta SO\ (eV)$	0.341	0.380	0.76	0.81		
$m_c^*\ (m_0)$	0.0670	0.0223	0.039	0.0135		
$EP\ (eV)$	28.8	21.5	27.0	23.3		
γ_1^L	6.98	20.00	5.18	34.8		
γ_2^L	2.06	8.50	1.19	15.5		
γ_3^L	2.93	9.20	1.97	16.5		
$a(\AA)$	5.6532	6.0583	4.4900	4.9850		
$C11\ (GPa)$	118.0	83.2	88.4	68.5	291.0	183.4
$C12\ (GPa)$	53.8	45.	40.3	37.4	155.5	122.6
$ac\ (eV)$	−7.17	−5.88	-7.5	-6.94	−2.20	−2.20
$av\ (eV)$	1.16	1.00	-0.8	-0.36	5.20	5.20
$b\ (eV)$	−1.70	−1.80	-2.0	-2.0	−2.20	−2.20

Table 2: Material parameters for zinc blende III-V compounds used in **k·p** calculations. Since incorporation of N is treated perturbatively, we do not require or provide band structure parameters for N-containing III-V binary compounds. The band gaps are given at T = 0 K; the room temperature band gaps are given in parentheses and were calculated using the Varshni parameters of Ref. [5].

	E_N(eV)	β (eV)	E_g(eV) (0 K)
GaAs	1.706	2.00	1.52
GaSb	0.77	2.40	0.78
InAs	1.386	1.212	0.42
InSb	0.720	1.97	0.23

Table 3: Values of isolated N energy states, E_N relative to valence band maximum energy, and BAC interaction parameter β, calculated using the sp^3s^* tight-binding model for the III-V compounds GaAs, GaSb, InAs and InSb, compared to low-temperature energy gap, E_g [from ref. 13].

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