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Composition dependence of the spin-orbit splittings in lattice-matched quaternary alloys: Generalized Van Vechten–Berolo–Woolley model

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We present a model including both inter- and intraband disorder-induced mixing which accounts for the recently observed composition dependence of the valence-band spin-orbit splittings Δ_0 and Δ_1 in the quaternary alloys InGaAsP and GaAlInAs lattice matched to InP.

The quaternary alloys when grown lattice matched to the substrate form an extremely interesting group of materials from both a fundamental and technological point of view. For example, they provide a testing ground for theories of random microscopic alloy disorder. In semiconductor alloys the change in crystal potential across the alloy field can be separated into two parts[1,2]: (1) a periodic part which is related to the change in lattice constant, and (2) an aperiodic part which is due to the random variations in the atomic potentials (alloy disorder). In lattice-matched quaternary alloy (LMOA) systems the lattice constant (bond length) is kept fixed (to that of the substrate material) and, hence, an important contribution to the change in the alloy crystal potential is eliminated. These quaternary alloys provide us with a system to measure directly the effects of aperiodicity.

It has been observed experimentally in semiconductor alloys that the energies of various interband transitions and spin-orbit splitting parameters vary quadratically with alloy composition,[1,2] i.e.,

$$E(x)=a+bx+cx^2 \tag{1a}$$

or

$$E(x)=a+b'x+cx(x-1)\ , \tag{1b}$$

where a and b' $(=b+c)$ are determined by the end-point material of the alloys series and c, the bowing parameter, measures the deviation from linearity.

It has been shown that the nonlinear composition dependence of various energies is a measure of the change in crystal potential (both periodic and aperiodic) across the alloy field.[1,2] However, in the LMQA systems the bowing coefficient is a manifestation of the microscopic aperiodicity only.[3,4]

In all ternary alloys having the zinc-blende structure it is found that[2] the bowing (a) for the spin-orbit splitting parameter Δ_0 (of the $\Gamma_{15,v}$ valence band) is downward, i.e., positive value of $c(\Delta_0)$ while (b) for Δ_1 (spin-orbit splitting of the $\Lambda_{3,v}$ valence bands) it is upward, i.e., negative value of $c(\Delta_1)$. However, recent studies of the quaternary alloys InGaAsP/InP (Refs. 3 and 5–8) and GaAlInAs/InP (Ref. 9) have reported negative values of $c(\Delta_0)$ as well as $c(\Delta_1)$. Listed in Table I are the values of a, b, and c for Δ_0 and Δ_1 for these systems as determined by several investigations. Note that for the InGaAsP/InP system, even though there is some variation in $c(\Delta_0)$, all the reported numbers are negative. We have also listed in Table I the average of the three values of a, b, and c for InGaAsP.

According to the Van Vechten–Berolo–Woolley (VV-B-W) model[2] a positive value of $c(\Delta_0)$ arises from an *interband* mixing of the s-like conduction-band states $(\Gamma_{1,c})$ into the p-like valence-band states $(\Gamma_{15,v})$ which effectively decreases Δ_0. This *interband* disorder-induced effect can be written as

$$\Delta_0(x)=[1-f(x)]\langle\Delta_0(x)\rangle\ , \tag{2}$$

where $\langle\Delta_0(x)\rangle=a+b'x$ [see Eq. (1b)]. The function $f(x)$ is the fraction of the conduction-band states mixed into the valence bands by alloy disorder and can be written as[2]

$$f(x)=D(x)/\bar{E}_0(x)\ , \tag{3}$$

where $D(x)$ is the mean-square fluctuation in crystal potential divided by an appropriate bandwidth, and $\bar{E}_0(x)$ is a

TABLE I. Values of the quadratic parameters a, b, and c for the spin-orbit splitting parameters Δ_0 and Δ_1 for $In_{1-y}Ga_yAs_xP_{1-x}$ and $(Ga_{1-x}Al_x)_{0.47}In_{0.53}As$ lattice matched to InP. All values were obtained at room temperature.

		a	b	c
		InGaAsP/InP		
Δ_0		0.114[a]	0.26[a]	−0.02[a]
		0.119[b]	0.30[b]	−0.107[b]
		0.11[c]	0.42[c]	−0.152[c]
	Average	0.114	0.327	−0.093
Δ_1		0.135[a]	0.33[a]	−0.20[a]
		0.145[b]	0.173[b]	−0.064[b]
		0.133[d]	0.124[d]	−0.07
	Average	0.138	0.209	−0.11
		GaAlInAs/InP		
Δ_0		0.37[e]	0.10[e]	−0.10[e]
Δ_1		0.28[e]	0.03[e]	−0.03[e]

[a]Reference 5.
[b]Reference 6.
[c]Reference 7.
[d]Reference 8.
[e]Reference 9.

weighted energy gap given by

$$\frac{3}{\bar{E}_0(x)} = \frac{2}{\langle E_0(x)\rangle} + \frac{1}{\langle E_0(x)+\Delta_0(x)\rangle} \quad . \tag{4}$$

In Eq. (4), $\langle E_0(x)\rangle$ and $\langle E_0(x)+\Delta_0(x)\rangle$ are the compositionally linear averaged energy gap and spin-orbit split component, respectively.

For the spin-orbit splitting of the Λ_3 valence bands, VV-B-W proposed a disorder induced *intraband* interaction which effectively increases Δ_1, i.e., the negative value for $c(\Delta_1)$. This term can be written as

$$\Delta_1(x) = \langle \Delta_1(x)\rangle + \frac{KD(x)}{\langle \Delta_1(x)\rangle} \quad , \tag{5}$$

where K is the factor which indicates the strength of the proposed selection rule for the disorder-induced fluctuating potential.

The negative value of both $c(\Delta_0)$ and $c(\Delta_1)$ for the quaternary alloys can be accounted for by including both *intra-* and *interband* effects for these spin-orbit splittings, thus generalizing the VV-B-W model. By including these two effects we can write

$$\Delta_i(x) = \langle \Delta_i(x)\rangle - \frac{D(x)}{\bar{E}_i(x)}\langle \Delta_i(x)\rangle + \frac{KD(x)}{\langle \Delta_i(x)\rangle} \quad , \tag{6}$$

where $i=0$ or 1. In the above expression, $\bar{E}_0(x)$ is given by Eq. (4) and $\bar{E}_1(x)$ by

$$\frac{2}{\bar{E}_1(x)} = \frac{1}{\langle E_1(x)\rangle} + \frac{1}{\langle E_1(x)+\Delta_1(x)\rangle} \quad . \tag{7}$$

For the quaternary alloy $In_{1-y}Ga_yAs_xP_{1-x}$ (Refs. 3 and 4),

$$D(x,y) = \frac{1}{A}[C^2_{\text{Ga-In}}y(1-y) + C^2_{\text{As-P}}x(1-x)] \quad , \tag{8}$$

where A is a bandwidth constant ($A \approx 1$ eV) and $C_{A\text{-}B}$ is the dielectrically defined electronegativity difference between elements A and B. Note that we have interchanged x and y in the usual notation for InGaAsP. The lattice-matched condition $x=2.2y$ plus values of $C^2_{\text{Ga-In}}$ and $C^2_{\text{As-P}}$ from Ref. 1 yields

$$D(x) = 0.07x + 0.149x(1-x) \quad . \tag{9}$$

In the case of the other quaternary system $(Ga_{1-x}Al_x)_yIn_{1-y}As$ the expression for $D(x,y)$ is given by

$$D(x,y) = \frac{1}{A}[C^2_{\text{Ga-Al}}xy(1-x) + C^2_{\text{Ga-In}}(1-x)(1-y)y + C^2_{\text{Al-In}}xy(1-y)] \quad . \tag{10}$$

For the lattice-matched system $y=0.47$; and hence

$$D(x) = 0.07 + 0.026x + 0.015x(1-x) \quad , \tag{11}$$

where we have used $C^2_{\text{Ga-Al}}$ and $C^2_{\text{Ga-In}}$ from Ref. 1 and $C^2_{\text{Al-In}}$ from Ref 4. In Eqs. (9) and (11) only the term containing $x(1-x)$ is relevant to calculate the bowing since the other terms are related to the end points.

We have used the generalized expression Eq. (6) to fit the $\Delta_0(x)$ and $\Delta_1(x)$ data for InGaAsP with Eq. (9) and GaAlInAs with Eq. (11) grown lattice matched to InP. The results for InGaAsP are displayed in Fig. 1. The solid lines

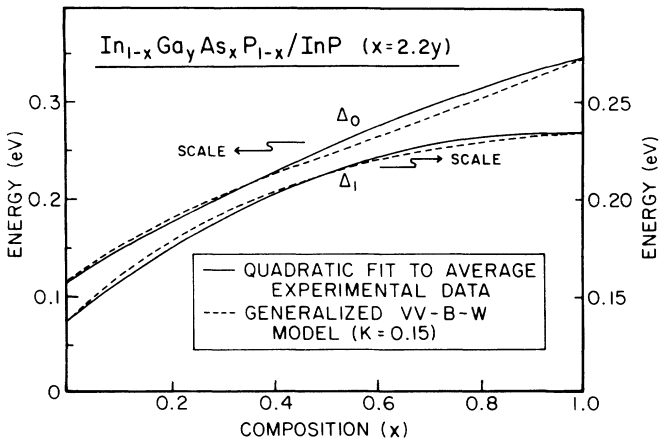

FIG. 1. Variation of the spin-orbit splittings with alloy composition x for $In_{1-y}Ga_yAs_xP_{1-x}$ lattice matched to InP ($x=2.2y$).

are given by the relation $E = a + bx + cx^2$, with a, b, and c for Δ_0 and Δ_1 being the average values listed in Table I. The dashed lines in Fig. 1 show the fit to the generalized VV-B-W model [Eqs. (6) and (9)]. We have adjusted the magnitude of the parameter K to get the best results for both $\Delta_0(x)$ and $\Delta_1(x)$ simultaneously, thus yielding a value of $K=0.15$. Note that the agreement between the average experimental values (solid lines) and the theory (dashed line) is good and the negative bowings of Δ_0 as well as Δ_1 have been accounted for. By considering only the *intra*band effect on the $\Delta_1(x)$ data, VV-B-W have obtained a value of $K=0.14$ for ternary alloys, while Kelso *et al.*[8] have found a value of $K=0.07$ for the InGaAsP system. Our value for K is close to that of VV-B-W but is somewhat larger than that quoted by Kelso *et al.*

Plotted in Fig. 2 are the compositional variation of $\Delta_0(x)$ and $\Delta_1(x)$ for GaAlInAs/InP. The solid lines represent a quadratic fit to the experimental points with the parameters (a,b,c) listed in Table I. The dashed lines again show the fit to these data using Eqs. (6) and (11). We obtained a value of $K=1.4$ for this quaternary alloy system. As for the InGaAsP system, the generalized VV-B-W model again accounts for the upward bowing of Δ_0 as well as Δ_1.

The variation in magnitude of K between the two alloy

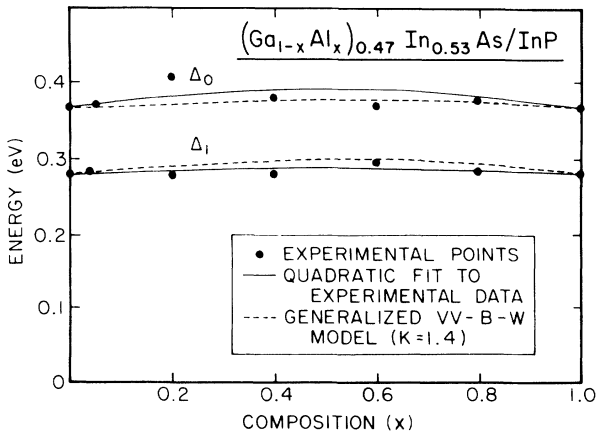

FIG. 2. Variation of the spin-orbit splittings with alloy composition x for $(Ga_{1-x}Al_x)_{0.47}In_{0.53}As$ lattice matched to InP.

systems is not completely understood at present. It may indicate the difference in strength of the proposed selection rule for the fluctuating potential, as pointed out by VV-B-W. For the $(Ga_{1-x}Al_x)_{0.47}In_{0.53}As$ alloy system, since the electronegativity difference of Ga and Al is small, we expect no significant deviation from linearity for both $\Delta_0(x)$ and $\Delta_1(x)$ [see Eq. (11)]. The fact that we observe an upward bowing for both $\Delta_0(x)$ and $\Delta_1(x)$ thus necessitating a larger value for K may suggest that there is more alloy disorder present in this system.

In conclusion, we have generalized the VV-B-W model to include both *inter-* and *intra*band effects. This generalized model successfully accounts for the upward bowing of Δ_0 found only in lattice-matched quaternary alloy systems, as well as the behavior of Δ_1. The difference in the magnitude of the parameter necessary to fit the data may indicate the different degree of microscopic alloy disorder in the two quaternary systems.

[1]J. A. Van Vechten and T. K. Bergstresser, Phys. Rev. B 1, 3351 (1970).

[2]J. A. Van Vechten, O. Berolo, and J. C. Woolley, Phys. Rev. Lett. 20, 1400 (1972); O. Berolo, J. C. Woolley, and J. A. Van Vechten, Phys. Rev. B 8, 3794 (1973).

[3]See, for example, T. P. Pearsall, *GaInAsP Alloy Semiconductors,* (Wiley, New York, 1982), Chap. 12.

[4]G. B. Stringfellow, J. Electron. Mater. 10, 919 (1981).

[5]P. M. Laufer, F. H. Pollak, R. E. Nahory, and M. A. Pollack, Solid State Commun. 36, 419 (1980).

[6]E. H. Perea, E. E. Mendez, and C. C. Fonstad, Appl. Phys. Lett. 36, 978 (1980).

[7]Y. Yamazoe, Ph.D. thesis (Osaka University, 1981) (unpublished).

[8]S. M. Kelso, D. E. Aspnes, M. A. Pollack, and R. E. Nahory, Phys. Rev. B 26, 6669 (1982).

[9]P. Parayanthal, C. S. Ro, F. H. Pollak, S. R. Stanley, G. W. Wicks, and L. F. Eastman, Appl. Phys. Lett. 43, 109 (1983).