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LETTER TO THE EDITOR

The effect of hydrostatic pressure on the band structure of the monolayer superlattice GaAs–$Ga_{1-x}Al_xAs(001)$

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Abstract. We have used an empirical tight-binding method to calculate the electronic band structure of the monolayer superlattice GaAs–$Ga_{1-x}Al_xAs$ as a function of composition ($0 < x < 1$) and hydrostatic pressure (0–50 kbar). We found that this empirical tight-binding method with a d^{-3} rule determining the off-diagonal matrix elements gives more accurate results for the energy gaps of GaAs, AlAs at high hydrostatic pressure which we also applied in the superlattice calculation. We believe that pressure coefficients are characteristic of symmetry structures for not only compounds like GaAs but also superlattices, and can be used to discern the origin of states, which is especially useful and convenient at high hydrostatic pressure where crossing of states may occur.

Using metal–organic chemical vapour deposition (MOCVD) and molecular beam epitaxy (MBE) growth methods, it is possible to grow GaAs–$Ga_{1-x}Al_xAs$ films as thin as one monolayer (Kawai *et al* 1984, Ishibashi *et al* 1985). Much work, both experimental and theoretical, has been done in investigating the electronic properties of such monolayer superlattices (MSL). However, the results usually contradict each other, e.g. the conduction band minima (CBM) given by different methods are different in both position and value (Schulman and McGill 1979, Andenoni *et al* 1978, Mon 1982, Wei and Zunger 1988, Zhang *et al* 1989). Using a developed empirical tight-binding method (DETBM: Vogl *et al* 1983), we studied the electronic band structure of MSL at atmospheric pressure and hydrostatic pressure and obtained some new results and conclusions on the nature of the CBM in MSL. The method we used has been discussed in existing literature (Vogl *et al* 1983, Mon 1982), but the following points should be noted.

One point is that we choose a 34:66 band offset which is now believed to produce more accurate and reasonable results than the previously used 15:85 band offsets (Wolford *et al* 1986). Another point is that by comparing calculated results and experimental data on GaAs and AlAs (table 1), we found that the results produced with a d^{-3} rule determining the off-diagonal matrix elements at high hydrostatic pressure are in much better agreement with those from Gell *et al* (1987) than results produced using a d^{-2} rule. Since the d^{-2} rule (Vogl *et al* 1983) is rather empirical and aimed mainly at giving a qualitative relationship among various compounds, it is not surprising that it does not accurately predict the band gaps of certain compounds such as GaAs at high hydrostatic pressure. Because GaAs and AlAs are the only constituents of the MSL of GaAs–$Ga_{1-x}Al_xAs$ and the interpolation scheme is still considered effective, we believe

Table 1. Calculated energies of the principal symmetry points in the lowest conduction bands of GaAs and AlAs obtained by three different methods. DETBM(2) and DETBM(3) indicate the DETBM with d^{-2} and d^{-3} rules, respectively, determining off-diagonal matrix elements under hydrostatic pressure. Data in the EPM column come from Gell *et al* (1987) and references therein.

P (kbar)	Samples	Γ_6^c EPM	Γ_6^c DETBM(3)	Γ_6^c DETBM(2)	X_6^c EPM	X_6^c DETBM(3)	X_6^c DETBM(2)
0	GaAs	1.523 (1.527)	1.550	1.550	2.012 (2.010)	2.030	2.030
	AlAs	3.020	3.040	3.040	2.290	2.300	2.300
10	GaAs	1.629 (1.629)	1.657	1.621	1.997 (1.997)	2.003	2.012
	AlAs	3.127	3.148	3.102	2.277	2.282	2.288
20	GaAs	1.737 (1.737)	1.758	1.690	1.984 (1.984)	1.977	1.995
	AlAs	3.235	3.253	3.181	2.263	2.266	2.277
30	GaAs	1.844 (1.844)	1.854	1.754	1.970 (1.970)	1.953	1.979
	AlAs	3.342	3.353	3.243	2.250	2.250	2.250
40	GaAs	1.951 (1.951)	1.942	1.816	1.956 (1.956)	1.930	1.964
	AlAs	3.449	3.452	3.308	2.236	2.235	2.256
50	GaAs	2.058 (2.058)	2.015	1.875	1.943 (1.943)	1.909	1.950
	AlAs	3.556	3.546	3.367	2.223	2.221	2.247
dE/dP	GaAs	10.6	10.4	6.5	−1.3	−2.4	−1.6
(meV kbar^{-1})	AlAs	10.2	10.3	6.6	−1.7	−1.7	−1.1

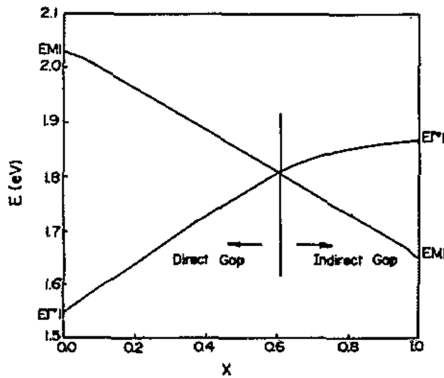

Figure 1. Variation with aluminium content x of the energies of EΓ1 and EM1 states.

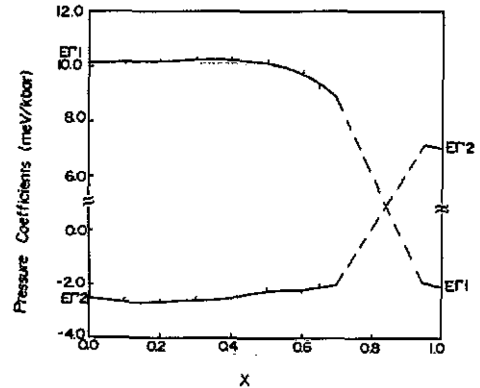

Figure 2. Variation with aluminium content x of pressure coefficients for EΓ1 and EΓ2 states. Dashed lines indicate the uncertain range and are guides for the eye.

that use of the d^{-3} rule is also practicable in MSL calculations. The third point is that the lattice constant a at any pressure is calculated according to the Murnaghan equation of state (Murnaghan 1944)

$$P = (B_0/B_0')[(V_0/V)^{B_0'} - 1]$$

where B_0 is the bulk modulus at $P = 0$ (we refer to atmospheric pressure as 0 kbar) and

Table 2. Energies for selected conduction states with respect to valence band maxima for MSL GaAs–AlAs and $Ga_{0.5}Al_{0.5}As$ alloy (in eV).

MSL	EΓ1	EΓ2	ER1	EM1
Our work	2.10	2.15	2.05	1.84
SM[a]	2.19	—	2.17	2.16
M[b]	≈1.97	—	—	≈1.95
ZHCGD[c]	2.11	2.23	1.85	2.13
Alloy	Γ_6^c	$X_{6,z}^c$	L_6^c	$X_{6,xy}^c$
Our work	2.29	2.17	2.20	2.17
ZHCGD	2.32	2.13	2.32	2.13

[a] Schulman and McGill (1979).
[b] Mon (1982).
[c] Zhang *et al* (1989).

Table 3. Pressure coefficients for two main symmetry states in MSL, $Ga_{0.5}Al_{0.5}As$ and GaAs.

Samples		State	Pressure coefficients (meV $kbar^{-1}$)
GaAs		Γ_6^c (X_6^c)	10.4 (−2.4)
AlAs		Γ_6^c (X_6^c)	10.3 (−1.7)
MSL	$x = 0.1$	EΓ1 (EΓ2)	10.2 (−2.5)
	$x = 0.2$	EΓ1 (EΓ2)	10.3 (−2.6)
	$x = 0.3$	EΓ1 (EΓ2)	10.4 (−2.5)
	$x = 0.4$	EΓ1 (EΓ2)	10.4 (−2.5)
	$x = 0.5$	EΓ1 (EΓ2)	10.3 (−2.1)
	$x = 0.6$	EΓ1 (EΓ2)	9.8 (−2.2)
	$x = 0.65$	EΓ1 (EΓ2)	9.3 (−1.9)
	$x = 0.7$	EΓ1 (EΓ2)	8.8 (−1.9)
	$x = 0.8$	EΓ1 (EΓ2)	7.5 (−1.9)
	$x = 0.8$–1.0	EΓ1 (EΓ2)	Unable to determine
	$x = 1.0$	EΓ1 (EΓ2)	−1.9 (7.2)

B_0' is the derivative of B_0 with respect to P. We use values of $0.755 + 0.026X$ Mbar and 4.49 (Adachi 1985, Gell *et al* 1987) respectively for B_0 and B_0'.

Our results indicate the following.

(i) At atmospheric pressure, GaAs–$Ga_{1-x}Al_xAs$ has an indirect gap between Γ(000) and M(100) when $x > 0.6$ (figure 1). The gap becomes narrower as x increases. When $x < 0.6$, GaAs–$Ga_{1-x}Al_xAs$ has a direct gap. The gap becomes larger as x increases. When $x = 0$, GaAs–$Ga_{1-x}Al_xAs$ becomes bulk GaAs with a direct gap of 1.55 eV. As examples, we list the energies of some selected conduction states for MSL GaAs–AlAs and $Ga_{0.5}Al_{0.5}As$ alloys in table 2, and compare them with previous results.

(ii) Pressure coefficients are characteristic of symmetry states for not only bulk compounds such as GaAs, but also for superlattices such as GaAs–$Ga_{1-x}Al_xAs$.

This conclusion—or, more precisely, this assumption—is based on two facts, together with our own calculation, illustrated to some extent in table 3 and figure 2. One fact is that the pressure coefficients for thick-layer superlattices $(GaAs)_n$–$(Ga_{1-x}Al_xAs)_m$

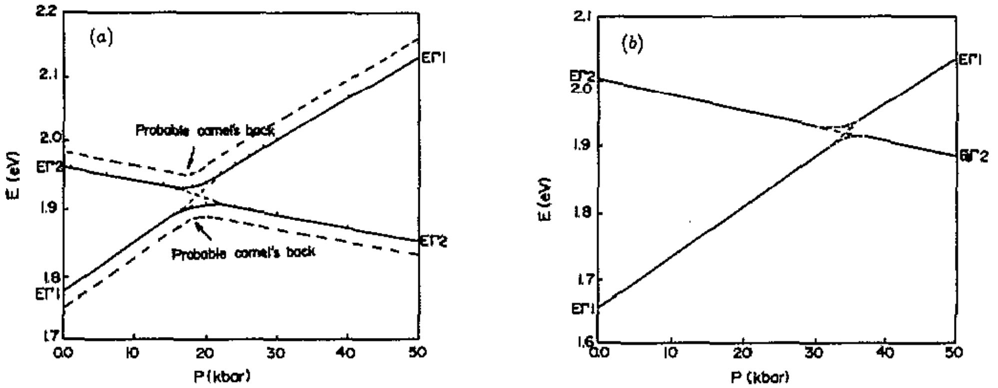

Figure 3. The effect of hydrostatic pressure on EΓ1 and EΓ2 states with (*a*) $x = 0.5$, (*b*) $x = 0.2$. Dashed lines are guides for the eye.

(TSL: $m, n > 10$) given by Gell *et al* (1987) are nearly equal to the corresponding data for bulk GaAs and AlAs. The other is a similar conclusion concerning bulk compounds drawn by Bassani and Kleinnan (1963), Bassani and Brust (1963) and Bassani and Parravicini (1975) after investigation of a great number of semiconductors. For instance, the pressure coefficients for Γ_6^c of many compounds range from 5 to 13 meV kbar^{-1}, and those for X_6^c range from -2 to 1 meV kbar^{-1}.

Using pressure coefficients, we can discern the origin of states, which is especially useful in MSL and TSL where there is a folding effect. For instance, from comparing pressure coefficients for EΓ1 and EΓ2 of MSL with those for Γ_6^c and X_6^c of bulk GaAs, AlAs and $Ga_{0.5}Al_{0.5}As$ (table 3 and figure 2), we know that when the aluminium composition $x \geqslant 0.9$, EΓ1 (we refer to the nth conduction state counted from the lowest conduction state at Γ as EΓn) is an X-related state (derived from an X_6^c state in bulk alloy), while it becomes Γ-related (derived directly from a Γ_6^c state in bulk alloy) when $x \leqslant 0.9$. It should be noted that because of the state mixing which we will discuss below, it is difficult to determine exactly the origin of EΓ1 and EΓ2 when x is around 0.9. However, our calculation shows that EΓ1 is X-related and EΓ2 is Γ-related when $x = 1.0$—that is, for the GaAs–AlAs superlattice.

Pressure coefficients for corresponding states can be either positive or negative—e.g. pressure coefficients for X or X-related states usually have a negative sign, while they are positive for Γ or Γ-related states. Thus, these states can cross at high hydrostatic pressure relatively more easily than in bulk compounds because of the narrower state gaps. If such crossing states are at the same symmetry point, e.g. EΓ1 and EΓ2, interaction between states occurs. Our calculation shows that this kind of state interaction happens when $|E\Gamma n - E\Gamma m| \leqslant 0.5$ eV (figure 3). Around this energy crossing level, states mix with each other and their energy levels change non-linearly, so the exact origin of these states will be of no significance at this stage. This is presumably the 'camel's back' in figure 11 in Gell *et al* (1987).

Because hydrostatic pressure does not change the symmetry of states, we can assume that the symmetry of states, and consequently the pressure coefficients for corresponding states, should remain unchanged as the state crossing reaches completion. Thus the changing direction of the states should remain nearly constant even at high hydrostatic

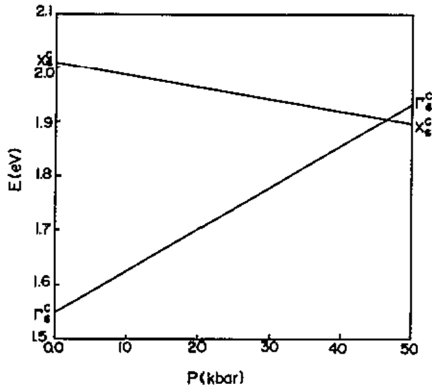

Figure 4. The effect of hydrostatic pressure on Γ_6^c and X_6^c states for bulk GaAs.

pressure, although convergence will be lost around the crossing level and the data there may be out of alignment. To show more evidence supporting this assumption, we present results on GaAs in figure 4, which we obtained by deliberately folding the bulk Brillouin zone into a tetragonal zone. Since such folding is in fact a pseudo-folding, interaction between states does not occur and the data for different states (Γ_6^c and X_6^c) are in perfect alignment.

Finally, we note that in bulk GaAs and TSL, which both have a direct gap, the CBM is a Γ or Γ-related state whose pressure coefficients are positive, while zone-edge states like X_6^c or EX1 usually have negative pressure coefficients. So the Γ–X crossing, namely the direct–indirect gap transition can take place at high hydrostatic pressure (Gell *et al* 1987). In GaAs–AlAs MSL, which has an indirect gap, on the other hand, the CBM is at M(100) where pressure coefficients are negative—the same sign as for EΓ1 which is X-related. Also, the pressure coefficients for GaAs–AlAs are smaller than the pressure coefficients for TSL (table 3); thus no Γ–M state crossing can occur. The same thing happens in $Ga_{0.5}Al_{0.5}As$ alloy, which can be analogously analysed.

In summary, we conclude that the d^{-3} rule is a better empirical rule for determining the off-diagonal matrix elements at high hydrostatic pressure; at least we believe that this is true for the calculations for GaAs, AlAs, $Ga_{1-x}Al_xAs$ and GaAs–$Ga_{1-x}Al_xAs$ superlattices. Pressure coefficients are characteristic of symmetry structures for both bulk compounds and superlattices. They are useful and convenient in discerning symmetries of states, especially at high hydrostatic pressure where state crossings may occur.

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