Comments

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Comment on "Spectroscopy of excited states in $In_{0.53}Ga_{0.47}As$-InP single quantum wells grown by chemical-beam epitaxy"

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Sauer *et al.* [Phys. Rev. B **34**, 9023 (1986)] have recently determined the band offsets of lattice-matched $In_{0.53}Ga_{0.47}As$-InP heterojunctions. We here show that the valence-band offset found by those authors (0.254 eV) agrees with that estimated by the dielectric-midgap-point method [M. Cardona and N. E. Christensen, Phys. Rev. B **35**, 6182 (1987)].

Sauer *et al.*[1] have recently measured the photoluminescence excitation spectrum of lattice-matched $In_{0.53}Ga_{0.47}As$-InP quantum wells. In these spectra two ladders of structures are seen which can be related to transitions from light- and heavy-hole subbands to the conduction subband of the same quantum number n. By fitting the energies of these structures to calculated values, they were able to determine the offsets of the valence- and conduction-band edges: The top of the valence band of InP was thus found to be 0.254 eV below that of $In_{0.53}Ga_{0.47}As$. In this Comment we show how to calculate this offset by combining the dielectric-midgap method[2] with the virtual-crystal approximation.

In the recent paper we have shown that the dielectric midgap energies (DME) obtained from linear muffin-tin orbitals (LMTO) band-structure calculations can be used to obtain band offsets between binary semiconductors.[2] The calculated DME's are brought together by the dielectric response of the interface until they nearly match. These produce a shift of the bands of one component with respect to the other which fixes the band offsets. Extensive tables of DME's, band-edge energies, and their volume coefficients have been published in Ref. 2. They can be used to calculate band offsets and their dependence on volume (i.e., pressure).

In order to estimate the band offsets in $In_{0.53}Ga_{0.47}As$-InP we must first estimate the DME and the band-edge energies of $In_{0.53}Ga_{0.47}As$. In the spirit of the virtual-crystal approximation we write any of these energies for an arbitrary ternary alloy $A_xB_{1-x}C$ as

$$E_i(x)=xE_i(AC)+(1-x)E_i(BC) +3x(1-x)[-a_i(AC)+a_i(BC)]\frac{\Delta a_0}{a_0}\ , \quad (1)$$

where the a_i's are the volume coefficients of the corresponding energies E_i and Δa_0 is the difference in the lattice constants of the AC and the BC compounds $[a_0(AC)-a_0(BC)]$. The band offset ΔE_v for the top valence-band states (Γ_8) of materials α and β is then[2]

$$\Delta E_v^{\alpha,\beta}=E_v^{\beta}-E_v^{\alpha}-(E_D^{\beta}-E_D^{\alpha})\frac{\bar{\epsilon}-1}{\bar{\epsilon}}\ , \quad (2)$$

where E_v^{α} (E_v^{β}) is the energy of the Γ_8 states of compounds α (β), E_D^{α} (E_D^{β}) the dielectric midgap energy and $\bar{\epsilon}$ an effective dielectric constant which can be taken to

TABLE I. Energies E_v, E_D and their volume coefficients a_v,a_D (in eV) required for the evaluation of the band offset ΔE_v of $In_{0.53}Ga_{0.47}As$-InP. Also, lattice constants a_0 (in Å) and dielectric constants $\bar{\epsilon}$ are listed.

	E_v	E_D	a_v	a_D	a_0	$\bar{\epsilon}$
InAs	−1.94	−1.32	−7.83	−7.82	6.05	12.3
GaAs	−1.07	−0.52	−8.77	−7.97	5.65	10.9
InP	−2.08	−1.21			5.86	9.6
$In_{0.53}Ga_{0.47}As$	−1.58	−0.95			5.86	11.6

be the average of the ir dielectric constants of α and β for $q=0$. If α is a ternary ($A_xB_{1-x}C$) we can take $\epsilon(\alpha)$ to be the weighted average of $\epsilon(AC)$ and $\epsilon(BC)$, where ϵ is the ir dielectric constant for $q=0$. The values of the parameters needed to evaluate Eq. (1) are listed in Table I (taken from Ref. 2) together with the energies E_v and E_D calculated with that equation for $In_{0.53}Ga_{0.47}As$. Using Eq. (2) we find from these energies and the corresponding ones for InP, $\Delta E_v=0.26$ eV, in good agreement with the value $\Delta E_v=0.254$ eV obtained experimentally in Ref. 1.

For a review of other measurements of this band offset the reader should see Ref. 3. While optical measurements yield values close to those discussed above, admittance spectroscopy data[3] yield $\Delta E_v=0.346\pm0.01$ eV. This value does not seem to be as satisfactory as that of Ref. 1 but would also be acceptable when compared with our theoretical estimate of 0.26 eV. Hence more work is required in order to elucidate the discrepancies between the various experimental estimates.

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[1]R. Sauer, T. D. Harris, and W. T. Tsang, Phys. Rev. B **34**, 9023 (1986).

[2]M. Cardona and N. E. Christensen, Phys. Rev. B **35**, 6182 (1987).

[3]D. V. Lang, M. B. Panish, F. Capasso, J. Allam, R. A. Hamm, and A. M. Sergent, Appl. Phys. Lett. **50**, 736 (1987).