NEW RELATIONS FOR BAND-EDGE OFFSETS IN LATTICE MATCHED HETEROJUNCTIONS

HRIVNÁK Ľ.,[1] Bratislava

Simple formulae for band-edge offsets in lattice-matched heterojunctions are proposed on the basis of an empirical correlation between the energy gap E_g^Γ, the lattice constant a, and the electron and light-hole effective masses m_e^Γ, m_{lh}^Γ at the Γ-point of semiconductors with zinc-blende structure: $E_g^\Gamma = (m_e^\Gamma + m_{lh}^\Gamma)\, c_g^2$, where $c_g = 2\pi\hbar/m_0 a$. In the most common lineup, when the energy gap difference at the interface equals the sum of the valence and conduction band discontinuities, $\Delta E_g^\Gamma = \Delta E_v^\Gamma + \Delta E_c^\Gamma$, we have proposed and verified the relations $\Delta E_v^\Gamma = \Delta m_{lh}^\Gamma c_g^2$ and $\Delta E_c^\Gamma = \Delta m_e^\Gamma c_g^2$.

I. INTRODUCTION

Any heterostructure is characterized by conduction and valence band discontinuities ΔE_c and ΔE_v, respectively, at the interface of the adjacent semiconductors. Various optical and electrical methods were elaborated for the experimental determination of these important parameters. However, there still remains the problem to calculate these parameters with sufficient accuracy. It was whown [1, 2, 3] that the simple Anderson rule in many cases fails and hardly any other simple rule exists which could be applicable to all heterostructures.

In this paper we confine ourselves to the problem of band discontinuities of lattice matched abrupt heterostructures with a *"straddling"* lineup when one forbidden band completely overlaps the other. The most investigated heterostructures and superlattices of this type are $GaAs/Al_xGa_{1-x}As$, $0 < x < 0.4$. For a review of various experimental results and theoretical approaches we recommend the papers by Dugan [4], Wang [5], Heinrich [6], Flores and Tejedor [7]. The related heterostructures which are nowadays of particular interest are $GaAs/Ga_{0.51}In_{0.49}P$ and $InP/In_{0.53}Ga_{0.47}As$. Theoretical approaches are usually compared with experimental data obtained on heterostructures of binary tetrahedrally coordinated $A^N B^{8-N}$ compounds.

[1] Institute of Electrical Engineering, Slovak Academy of Sciences, Dúbravská cesta 9, CS-842 39 BRATISLAVA, Czechoslovakia

II. THE EMPIRICAL RULE FOR THE BANDWIDTHS

Suppose that in semiconductors the k-dependence of the electron energy in the conduction band with respect to the bottom of the conduction band ($E_c = 0$) can be approximated by the relation

$$\frac{\hbar^2 k^2}{2m_e^\Gamma} = E(k)\,(1 + aE(k)), \tag{1}$$

where m_e^Γ is the electron effective mass at the bottom of the conduction at $k = 0$ (Γ-point) and a is the nonparabolicity coefficient. The relation (1) can be rewritten into the "relativistic" for

$$E^{*2}(k)/c_g^2 = p^2 + m_e^{\Gamma 2} c_g^2, \tag{2}$$

where $p^2 = \hbar^2 k^2$,

$$E^*(k) = E(k) + m_e^\Gamma c_g^2 \tag{3}$$

and

$$c_g^2 = 1/2m_e^\Gamma a. \tag{4}$$

With $k = 0$ the relation (3) gives

$$E_c^\Gamma = m_e^\Gamma c_g^2. \tag{5}$$

Suppose that with the same zero energy level the value of the top of a valence band at the Γ-point is

$$E_v^\Gamma = -m_{lh}^\Gamma c_g^2, \tag{6}$$

where m_{lh}^Γ is the light hole effective mass at the top of the valence band. Then the energy band gap at the Γ-point is

$$E_g^\Gamma = E_c^\Gamma - E_v^\Gamma = (m_e^\Gamma + m_{lh}^\Gamma)\, c_g^2, \tag{7}$$

which resembles the well-known relation for the minimal energy necessary for the creation of an electron-positron pair,

$$E_0 = 2m_0 c^2,$$

m_0 and c being the electron rest mass and the light velocity, respectively. Taking $m_{lh}^\Gamma \approx m_e^\Gamma$ we have shown previously [8] that the relation (7) is approximately fulfilled for many $A^N B^{8-N}$ crystals with zinc-blende structure if

$$c_g = 2\pi\hbar/am_0, \tag{8}$$

which is the group velocity of a free electron with the de Broglie wave-length equal to the lattice constant a.

The relation (8) follows from Heisenberg's uncertainty relation

$$\Delta x \Delta p_x = 2\pi\hbar$$

if we take as the minimal uncertainty of the conduction electron position $\Delta x = a$ and the corresponding maximum uncertainty of the electron momentum $\Delta p_x = m_0 c_g$. A verification of the relation (7) with c_g given by (8), i.e.

$$\frac{E_g^\Gamma a^2}{(m_e^\Gamma + m_{lh}^\Gamma)/m_0} = \frac{h^2}{m_0} \tag{9}$$

is shown in Table 1. On the left side of the equality (9) there are measurable parameters of a given tetrahedrally coordinated crystal with a diamond or a

Table 1

Verification of the relation $(m_e^\Gamma + m_{lh}^\Gamma)/m_0 = a^2 m_0 E_g^\Gamma/h^2$ using the values of E_g^Γ, m_e^Γ/m_0 and m_{lh}^Γ/m_0 calculated by Lawaetz [23].

Crystal	a (10^{-10} m)	E_g^Γ (eV)	m_e^Γ/m_0	m_{lh}^Γ/m_0	$(m_e^\Gamma + m_{lh}^\Gamma)/m_0$	$a^2 m_0 E_g^\Gamma/h^2$
InSb	6.479	0.237	0.014	0.015	0.029	0.033
InAs	6.058	0.42	0.023	0.027	0.050	0.051
GaSb	6.095	0.81	0.045	0.046	0.091	0.100
Ge	5.657	0.89	0.038	0.043	0.081	0.095
InP	5.869	1.42	0.080	0.089	0.169	0.162
GaAs*	5.653	1.52	0.067	0.074	0.141	0.161
CdTe	6.477	1.60	0.096	0.103	0.199	0.223
AlSb	6.135	2.30	0.18	0.14	0.32	0.288
ZnTe	6.101	2.39	0.18	0.154	0.334	0.295
ZnSe	5.667	2.82	0.14	0.149	0.289	0.301
GaP	5.450	2.87	0.17	0.14	0.31	0.283
AlAs	5.662	3.06	0.22	0.15	0.37	0.326
Si	5.431	4.07	0.23	0.16	0.39	0.399

* According to Blakemore [18] in GaAs at 300 K $E_g^\Gamma = 1.423$ eV, $m_e^\Gamma/m_0 = 0.0632$, $m_{lh}^\Gamma/m_0 = 0.088$, $a = 5.65325 \times 10^{-10}$ m. Then $a^2 m_0 E_g/h^2 = 0.15117$ and $(m_e^\Gamma + m_{lh}^\Gamma)/m_0 = 0.1512$.

zinc-blende structure while on the right-hand side there are only universal constant. No other empirical parameters enter the relation (9). Yet we should consider it as an empirical relation, since we are not able to derive it from first principles. The relation (9) can be rewritten as

$$E_g^\Gamma = 3\pi^2\hbar^2(m_e^\Gamma + m_{lh}^\Gamma)/4m_0^2 d^2, \tag{10}$$

where $d = \sqrt{3}\,a/4$ is the nearest-neighbour distance in tetrahedrally cordinated crystals with zinc-blende structure. This relation gives the same dependence of E_g^Γ on the nearest-neighbour distance d as the previously known empirical rule for the optical bandwidth of tetrahedral and also rock-salt crystals which Pantelides [9] introduced in the form

$$E_g^\Gamma = \eta_g \hbar^2/m_0 d^2. \tag{11}$$

Here the "band-gap index" η_g is an empirical constant which in rock-salt crystals depends on the chemical valence of the constituent atoms. Adachi [10] pointed out the linear dependence of m_e^Γ and m_{lh}^Γ on the lowest-direct gap E_g^Γ for some III—V binaries, which is inherent in our relation.

III. NEW RELATIONS FOR BAND-EDGE OFFSETS

Suppose that a heterostructure consists of two semiconductors with different energy gaps, $E_{g1}^\Gamma > E_{g2}^\Gamma$, but an approximately equal lattice constant. Using the relations

$$\begin{aligned} E_{g1}^\Gamma &= (m_{e1}^\Gamma + m_{lh1}^\Gamma)\, c_g^2 \\ E_{g2}^\Gamma &= (m_{e2}^\Gamma + m_{lh2}^\Gamma)\, c_g^2 \end{aligned} \tag{12}$$

we can express the energy gap difference $\Delta E_g^\Gamma = E_{g1}^\Gamma - E_{g2}^\Gamma$ as

$$\Delta E_g^\Gamma = (m_{e1}^\Gamma - m_{e2}^\Gamma + m_{lh1}^\Gamma - m_{lh2}^\Gamma)\, c_g^2. \tag{13}$$

The band-edge discontinuities at the interface ΔE_c^Γ, ΔE_v^Γ in the case of a straddling lineup should fulfil the relation

$$\Delta E_g^\Gamma = \Delta E_c^\Gamma + \Delta E_v^\Gamma. \tag{14}$$

Since according to the relation (13) ΔE_g^Γ depends on the electron and the light-hole effective masses of semiconductors forming the lattice-matched heterostructure, the relation (14) should be fulfilled by properly chosen functions ΔE_c^Γ, ΔE_v^Γ of the same set of the effective masses. We have chosen the functions

$$\Delta E_v^\Gamma = (m_{lh1}^\Gamma - m_{lh2}^\Gamma)\, c_g^2 \tag{15}$$

$$\Delta E_c^\Gamma = (m_{e1}^\Gamma - m_{e2}^\Gamma)\, c_g^2. \tag{16}$$

A schematic representation of the proposed relations is shown in Fig. 1. Our zero "mid-gap" energy level is constant across the heterostructure.

The band-edge offsets for the considered heterostructures are given as differences between quantitites which are intrinsic to constituent bulk materials.

The results can be generalized to structures consisting of the several layers with a common "midgap" zero energy level. In this case the commutative and transitive rules are obviously fulfilled:

$$\Delta E^{\Gamma}_{c13} = \Delta E^{\Gamma}_{c12} + \Delta E^{\Gamma}_{c23}. \tag{17}$$

Thus, our formulae for heterostructures with a straddling lineup obey the general rules demanded by both experiment [11] and theory [7, 12].

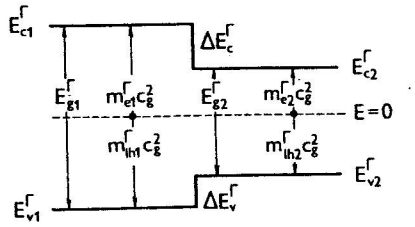

Fig. 1. Schematic band diagram of a lattice-matched abrupt heterostructure which corresponds to relations (15) and (16).

IV. COMPARISON WITH EXPERIMENT

Let us apply the formula (16) to the experimentally most investigated GaAs/$/Al_xGa_{1-x}As$ heterostructures. In this case $a = 0.5633$ nm, $m_0c_g^2 = 9.4$ eV. The composition dependence of the energy gap and the electron effective mass for $x < 0.4$ can be approximated as [10]

$$E^{\Gamma}_g(x) = (1.423 + 1.247x)\,\text{eV} \tag{18}$$

and

$$m^{\Gamma}_e(x)/m_0 = 0.067 + 0.083x, \tag{19}$$

respectively. Then, the relation (16) gives

$$\Delta E^{\Gamma}_c = 0.78x\,\text{eV} = 0.63\Delta E^{\Gamma}_g \tag{20}$$

in very good accordance with recent experimental results obtained by various authors and methods [13, 14, 15, 16].

Wolford et al. [16] published the result of very precise measurements of ΔE^{Γ}_v of both direct and indirect gap GaAs/$Al_xGa_{1-x}As$ heterostructures. Their results can be fitted by the relation

$$\Delta E^{\Gamma}_v = (0.350x + 0.153x^2)\,\text{eV} \tag{21}$$

for the whole composition range $0 \le x \le 1$. Using the relation

$$\Delta E^{\Gamma}_g = (1.155x + 0.37x^2)\,\text{eV} \tag{22}$$

in accordance with Lee et al. [17] and the relation (14) we obtain

$$\Delta E^{\Gamma}_c = (0.805x + 0.217x^2)\,\text{eV}, \tag{23}$$

which corresponds very well to the experimental results obtained by Okumura et al. [13]. The above relations yield a 68/32 conduction to valence-band discontinuities ratio.

Using our relations (15) and (16) with $m_0c_g^2 = 9.4$ eV and the room temperature values of the electron and the light-hole effective masses in GaAs equal to $0.0632m_0$ and $0.088m_0$ [18], respectively, the relations (21) and (23) give

$$m^{\Gamma}_{lh}(x)/m_0 = 0.088 + 0.0372x + 0.0163x^2, \tag{24}$$

$$m^{\Gamma}_e(x)/m_0 = 0.0632 + 0.856x + 0.0231x^2. \tag{25}$$

The plots of these functions are shown in Fig. 2. Notice that in the region of x for which $Al_xGa_{1-x}As$ is an indirect gap semiconductor, there is $m^{\Gamma}_e(x) > m^{\Gamma}_{lh}(x)$, similarly as in other indirect gap semiconductors (see Table 1). Our estimation of the electron and the light-hole effective masses on the basis of our formulae for band-edge offsets and their experimental values in GaAs/

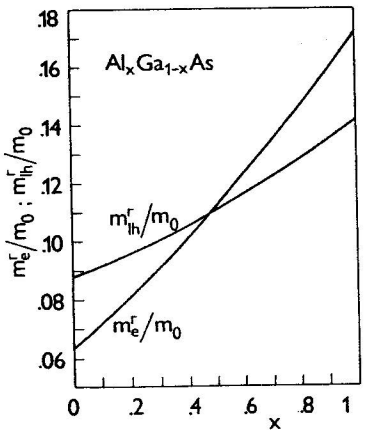

Fig. 2. Conduction electron and light-hole effectice masses at the Γ-point of $Al_xGa_{1-x}As$ as a function of the composition deduced from observed band-edge offsets by the use of the relations (15) and (16).

$Al_xGa_{1-x}As$ heterostructures is a new one. It should be verified by independent experimental methods.

The relations (15) and (16) with $m_0c_g^2 = 9.4$ eV and $m_e^\Gamma(x)/m_0$, $m_{lh}^\Gamma(x)/m_0$ given by (24) and (25), respectively, enable to construct Fig. 3 for $GaAs/Al_xGa_{1-x}As$ heterostructures, where $\Delta E_v^\Gamma(x)$, $\Delta E_c^\Gamma(x)$ are given by the relations (21) and (23). Obviously the relations (14) and (22) are fulfilled, too. Some experimental data are also displayed in this figure. This figure illustrates how the values of $m_e^\Gamma(x)$ and $m_{lh}^\Gamma(x)$ can be determined when the experimental values of $\Delta E_c^\Gamma(x)$ and $\Delta E_v^\Gamma(x)$ are known from experiment and the relation (14) holds.

Recently, the valence-band offset in $GaSb/Al_xGa_{1-x}Sb$ quantum wells has been determined by Menéndez et al. [19] by the light scattering method at

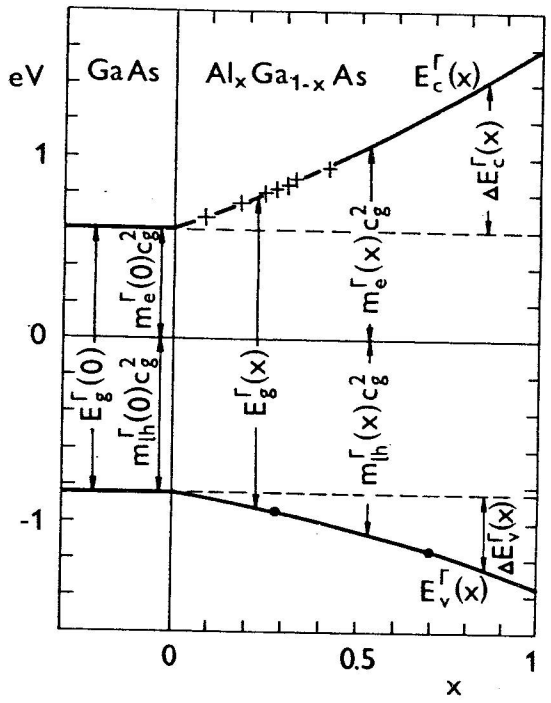

Fig. 3. Composition dependences of valence and conduction band discontinuities of $Al_xGa_{1-x}As/GaAs$ heterojunctions in accordance with the relations (21) and (23). The crosses denote the experimental results obtained by Okumura et al. [13] and the dots correspond to the experimental values of ΔE_v^Γ obtained by Wolford et al. [16]. The values of $m_{lh}^\Gamma(x)c_g^2$ and $m_e^\Gamma(x)c_g^2$ rorrespond to the relations (26) and (27), respectively, and $m_0c_g^2 = 9.4$ eV.

liquid helium temperature as

$$\Delta E_v^\Gamma = (0.45 \pm 0.08)\,x \text{ eV}. \tag{26}$$

For $x = 0.114$ these authors found $\Delta E_c^\Gamma = 0.0829$ eV, $\Delta E_v^\Gamma = 0.0516$ eV, $\Delta E_g^\Gamma = 0.1345$ eV. With lattice constants from Table 1 we obtain the values of $m_0c_g^2$ equal to 8.075 eV and 7.971 eV for GaSb and AlSb, respectively. Using the value of $m_0c_g^2 = 8.0$ eV for $Al_xGa_{1-x}Sb$ and the light-hole effective mass in GaSb determined by Stradling [20] at 20 K, $m_{lh}^\Gamma/m_0 = 0.052$, we obtain from (26) on the basis of the relation (15)

$$m_{lh}^\Gamma(x)/m_0 = 0.052 + 0.056x. \tag{27}$$

Using the relation

$$\Delta E_g^\Gamma(x) = (1.129x + 0.368x^2)\text{ eV} \tag{28}$$

in accordance with Casey and Panish [21] and the relations (14) and (26) we get

$$\Delta E_c^\Gamma = (0.679x + 0.368x^2)\text{ eV}. \tag{29}$$

By comparison with the relation (15) we obtain

$$m_e^\Gamma(x)/m_0 = 0.047 + 0.0849x + 0.046x^2, \tag{30}$$

where we have used the experimental value of the electron effective mass in GaSb determined by Braunstein and Kane [22]. This relation gives the value of the electron effective mass at the Γ-point in AlSb as equal to $0.178m_0$, which is close to the value calculated by Lawaetz [23]. The value of m_{lh}^Γ/m_0 for AlSb following from (27) is 0.108 in accordance with the experimental value $m_{lh}^\Gamma/m_0 = 0.11$ determined by Cardona et al. [24]. For $x = 0.114$ we obtain on the basis of the relations (16), (27), (30) and $m_0c_g^2 = 8.0$ eV the results: $\Delta E_c^\Gamma = 0.0822$ eV, $\Delta E_v^\Gamma = 0.0510$ eV, in good accordance with the above introduced experimental results by Menéndez et al. [19].

Another lattice-mattched direct-gap heterojunction for which there are reliable experimental results recently published by Rao et al. [25], is $Ga_{0.51}In_{0.49}P/GaAs$. According to these authors $\Delta E_v^\Gamma = 0.239\text{ eV} = 0.52\,\Delta E_g^\Gamma$, $\Delta E_c^\Gamma \approx 0.22\text{ eV} \approx 0.48\,\Delta E_g^\Gamma$, $\Delta E_g^\Gamma = \Delta E_v^\Gamma + \Delta E_c^\Gamma = 0.459$ eV, the energy gaps in $Ga_{0.51}In_{0.49}P$ and GaAs being 1.883 eV and 1.424 eV, respectively. Taking the values of the electron and the light-hole effective masses in GaAs 0.0632 and $0.088m_0$ we obtain from (16) for $Ga_{0.51}In_{0.49}P$ the values: $m_e^\Gamma/m_0 = 0.0865$ and $m_{lh}^\Gamma/m_0 = 0.1135$, when $m_0c_g^2 = 9.4$ eV is used.

As a further example of application of our formulae we give InSb/CdTe

heterojunction. Using the values $a = 0.6479$ nm, $E_g^\Gamma = 0.23$ eV, $m_e^\Gamma/m_0 = 0.016$ for InSb and $a = 0.6479$ nm, $E_g^\Gamma = 1.60$ eV, $m_e^\Gamma/m_0 = 0.100$ for CdTe, we obtain $\Delta E_c^\Gamma = 0.603$ eV, $\Delta E_v^\Gamma = 0.77$ eV, in accordance with the values computed by Van Walzenis and Vredenbregt [26]. Experimental value of ΔE_v^Γ is (0.87 ± 0.10) eV [27].

V. COMPARISON OF OUR RESULTS WITH OTHER ESTIMATION OF BAND-EDGE OFFSETS

As we have shown on several examples, in case of a straddling lineup the knowledge of the lattice constant and the electron and light-hole effective masses as the Γ-point of crystals with zinc-blende structure enables us to calculate the energy gaps and both the conduction and the valence band-edge discontinuities. The well-known Anderson rule enables (in some cases) to determine only the conduction band-edge offset as a difference of the electron affinities of the corresponding semiconductors:

$$\Delta E_c = \Delta\chi. \tag{31}$$

Tersoff [29] introduced an energy E_B associated with each semiconductor which represents the energy (usually deep in the gap) where the states are non-bonding on the average. The condition of the continuity of E_B (given relative to valence band-edge E_v) across the inference implies

$$\Delta E_v = -\Delta E_B. \tag{32}$$

Recently Jaros [30] has shown that a valence band-edge discontinuity can be estimated from a simple relation, which requires only the knowledge of the lattice constant and the relative optical permittivity of the corresponding crystals with a diamond or a zinc-blende structure:

$$\Delta E_v = \Delta\langle E_g\rangle, \tag{33}$$

where $\langle E_g\rangle$ is determined by the relation

$$\epsilon_\infty = 1 + (\hbar\omega/\langle E_g\rangle)^2,$$

$\omega = (ne^2/\epsilon_0 m_0)^{1/2}$ is the plasma frequency, n is the electron density which in diamond or zinc-blende crystals is $32/a^3$.

In Table 2 the parameters for some semiconductors are given which are necessary for band-edge offsets estimations according to Anderson's rule, Tersoff's theory, Jaros's estimation and our empirical formulae. The results for

Table 2

The parameters of some semiconductors which are necessary for band-edge offsets estimations according to the relations (15) and (16), (31), (32), (33).

Crystal	m_e^Γ/m_0	m_{lh}^Γ/m_0	$m_0c_g^2$ [eV]	χ [eV] [28]	E_B [eV] [29]	$\langle E_g\rangle$ [eV] [30]
GaAs	0.0632	0.088	9.4	4.07	0.50	4.97
AlAs	0.172	0.1415	9.4	3.5	1.05	5.82
GaSb	0.040	0.048	8.0	4.06	0.07	3.80
AlSb	0.178	0.108	8.0	3.65	0.45	4.56
InSb	0.014	0.015	7.15	4.59	0.01	3.33
CdTe	0.096	0.128	7.15	4.28	0.85	5.11

Table 3

Comparison of various band-edge offsets estimations.

eV	Heterostructures		
	AlAs/GaAs	AlSb/GaSb	CdTe/InSb
ΔE_g^Γ (13)	1.528	1.584	1.379
ΔE_c^Γ (16)	1.025	1.104	0.571
ΔE_c^Γ (15)	0.503	0.480	0.808
ΔE_v^Γ exp	0.45—0.55 [4]	0.45 [19]	0.87 ± 0.1 [27]
ΔE_v^Γ [29]	0.55	0.38	0.84
ΔE_v^Γ [30]	0.43	0.38	0.89
ΔE_v^Γ [31]	0.60	0.43	—
ΔE_v^Γ [32]	0.43	0.34	0.66
$\Delta\chi$	0.57	0.41	0.29

various lattice-matched hetrostructures are displayed in Table 3 together with the values calculated by Van de Walle and Martin [31], Cardona and Christensen [32], and the experimental values of ΔE_v^Γ.

VI. CONCLUSION

We have shown that our relations (13), (15) and (16) enable us to estimate the values of ΔE_g^Γ, ΔE_v^Γ and ΔE_c^Γ at the interface of lattice-matched heterostructures in the case when one forbidden band completely overlaps the other. We need to know only the lattice constant and the electron and light-hole effective masses of the constituent materials. The relation (13) follows directly from an empirical

relation (9) for the energy gap at the Γ-point of the crystal with a zinc-blende structure. The relations (15) and (16) are valid due to the band lineup shown in Fig. 1. The proposed relations should be considered as empirical, since they have not been proved on the basis of a rigorous theory, but deduced from experimental data. If the band gaps and the band-edge offsets fulfilling the relation (14) are experimentally well established, then our relations enable us to estimate the values of the electron and the light-hole effective masses, as we have shown for the $Al_xGa_{1-x}As/GaAs$ heterostructures.

REFERENCES

[1] Bauer, R. S., Zurcher, P., Sang, H. W.: Appl. Phys. Lett. *43* (1983), 663
[2] Milnes, A. G.: Solid State Electronics *29* (1986), 99
[3] Niles, D. W., Margaritondo, G.: *18th Internat. Conf. on the Physics of Semiconductors.* Stockholm 1986, Editor Engström, O., World Scientific, vol. 1, p. 187
[4] Duggan, G.: J. Vac. Sci. Technol. *B3* (1985), 1224
[5] Wang, W. I.: Solid State Electronics *29* (1986), 133
[6] Heinrich, H.: Acta Phys. Polonica *A71* (1987), 125
[7] Flores, F., Tejedor, C.: J. Phys. C: Solid State Phys. *20* (1987), 145
[8] Hrivnák, L.: Czech. J. Phys. *B35* (1985), 581
[9] Pantelides, S. T.: Phys. Rev. *B12* (1975), 5082
[10] Adachi, S.: J. Appl. Phys. *58* (1985), R1
[11] Katnani, A. D., Bauer, R. S.: Phys. Rev. *B33* (1986), 1106
[12] Van de Walle, Ch. G., Martin, R. M.: as in ref. [3], p. 159
[13] Okumura, H., Misawa, S., Yoshida, S., Gonda, S.: Appl. Phys. Lett. *46* (1985), 377
[14] Batey, J., Wright, S. L., DiMaria, D. J.: J. Appl. Phys. *57* (1985), 484
[15] Hill, A. J., Ladbrooke, P. H.: Electronic Letters *22* (1986), 218
[16] Wolford, D. J., Kuech, T. F., Bradley, J., Gell, M. A., Ninno, D., Jaros, M.: J. Vac. Sci. Technol. *B4* (1986), 1043
[17] Lee, H. J., Juravel, L. Y., Wooley, J. C.: Phys. Rev. *B21* (1980), 659
[18] Blakemore, J. S.: J. Appl. Phys. *53* (1980), R123
[19] Menéndez, J., Pinczuk, A., Werder, D. J., Valladares, J. P., Chiu, T. H., Tsang, W. T.: Solid State Commun. *61* (1987), 703
[20] Stradling, R.: Phys. Lett. *20* (1966), 217
[21] Casey, H. C. Jr., Panish, M. B.: *Heterostructures Lasers Part B: Materials and Operating Characteristics.* New York, Academic 1978, p. 16
[22] Braunstein, R., Kane, E.: J. Phys. Chem. Solids *23* (1962), 1423
[23] Lawaetz, P.: Phys. Rev. *B4* (1971), 3460
[24] Cardona, M., Pollak, F. H., Shaklee, K. L.: Phys. Rev. Lett. *16* (1966), 644
[25] Rao, M. A., Caine, E. J., Kroemer, H., Long, S. I., Babic, D. I.: J. Appl. Phys. *61* (1987), 643
[26] Welzenis, Van R. G., Vredenbregt, J. D.: Solid State Electronics *28* (1985), 1057
[27] Mackey, K. J., Allen, P. M. G., Herrenden-Harker, W. G., Williams, R. H.: Appl. Phys. Lett. *49* (1986), 354
[28] Milnes, A. G., Feucht, D. L.: *Heterojunctions and Metal-Semiconductor Junctions.* New York, Academic 1973, Table 1.3

[29] Tersoff, J.: J. Vac. Sci. Technol. *B4* (1986), 1066
[30] Jaros, M.: Phys. Rev. *B37* (1988), 7112
[31] Van de Walle, C. G., Martin, R. M.: J. Vac. Sci. Technol. *B4* (1986), 1055
[32] Cardona, M., Christensen, N. E.: Phys. Rev. *B35* (1987), 6182

Received June 28th, 1988
Accepted for publication July 12th, 1988

НОВЫЕ СООТНОШЕНИЯ ДЛЯ РАЗРЫВОВ В ЗОНАХ В РЕШЕТОЧНО-СОГЛАСОВАННЫХ ГЕТЕРОПЕРЕХОДАХ

Предложена простая формула для разрывов в зонах в решеточносогласованных гетеропереходах на основе эмпирических корреляций между энергией шели E_g^Γ, постоянной решетки a, и эффективными массами электрона и дырки m_e^Γ, m_{lh}^Γ, в Γ-точке полупроводника со структурой цинковой обманки: $E_g^\Gamma = (m_e^\Gamma + m_{lh}^\Gamma)\, c_g^2$, где $c_g = 2\pi\hbar/m_0 a$. В самой общей расстановке, когда разница энергий на границе раздела равна сумме разрывов зон, $\Delta E_g^\Gamma = \Delta E_v^\Gamma + \Delta E_c^\Gamma$, мы предложили и проверили соотношения $\Delta E_v^\Gamma = \Delta m_{lh}^\Gamma c_g^2$, $\Delta E_c^\Gamma = \Delta m_e^\Gamma c_g^2$.