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Citation: Applied Physics Letters **58**, 1056 (1991); doi: 10.1063/1.104421
View online: http://dx.doi.org/10.1063/1.104421
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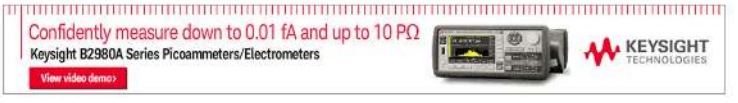

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Band offset in $InP/Ga_{0.47}In_{0.53}As$ heterostructures

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(Received 1 August 1990; accepted for publication 10 December 1990)

Energy levels in $InP/Ga_{0.47}In_{0.53}As$ quantum wells are calculated after reformulating the energy-dependent effective mass to be used for taking into account the energy-band nonparabolicity of both constituents. The required value of the ratio of the conduction-band and valence-band discontinuities is found to be close to 2/3, in agreement with the value found by other methods. The value of the nonparabolicity factor is also found to be the same as that used in earlier transport studies.

The $InP/Ga_{0.47}In_{0.53}As$ quantum wells are being studied extensively, as the high electron mobility in $Ga_{0.47}In_{0.53}As$ promises high-speed devices. One important parameter of this system is the ratio of the conduction-band discontinuity, ΔE_c, and the energy-gap discontinuity, ΔE_g, at the interfaces. Values derived for this parameter by different methods, however, do not agree and range between 0.25 and 0.65.[1–11] One method which has been extensively used, is the comparison of calculated values with experimental results on energy shift[12–15] in photoluminescence experiments. All other constants being known, the conduction-band discontinuity is chosen to fit the experimental results. The energy-band nonparabolicity is reported to be important in determining the position of the energy level and this parameter has also been derived[3] in some studies from analysis of photoluminescence data. The band nonparabolicity has, however, been treated in different ways by different workers[16–18] and there is no agreement in the literature about its effect on the energy levels. The purpose of this letter is to discuss this aspect of the problem and to reanalyze the published data to deduce a value of band-edge discontinuity.

Energy levels for the quantum wells are evaluated by solving the Schrödinger equation with the effective mass formalism, written below:

$$\left(\frac{\hbar^2}{2m_i^*}\right)\left(\frac{d^2\psi_i}{dz^2}\right)+(E-E_{ci})[1+\alpha_i(E-E_{ci})]\psi_i=0, \quad (1)$$

where m_i^* is the effective mass at the band edge, E_{ci}, E is the energy, α_i is the nonparabolicity parameter[19] and ψ_i is the wave function, i being the subscript to indicate the well or the barrier layer. It should be noted that this formalism has been used even for wells a few monolayers thick. Distinct photoluminescence peaks with 1.2 meV full width half maximum (FWHM) are obtained with such layers and it is estimated[20] that the interface is distinct to within $0.12a_0$ (a_0 is the lattice constant). This result indicates that the energy-band concept remains valid, but whether the energy bands remain the same as in bulk is not clear. In the absence of any indication to the contrary, analysis is extended in this note down to such narrow wells with the bulk effective mass. Solution of the above equation is

$$\psi_i=A_i\exp(ik_iz)+B_i\exp(-ik_iz), \quad (2)$$

where

$$k_i^2=(2m_i^*/\hbar^2)(E-E_{ci})[1+\alpha_i(E-E_{ci})]. \quad (3)$$

It may be noted that k_i is real in the well layer, but in the barrier layer it is imaginary for the confinement energies.

The constants A_i and B_i are required to be obtained by applying the boundary conditions,

$$\text{(i) } \psi_B=0 \text{ for } |z|\to\infty; \quad (4)$$

$$\text{(ii) } \psi_W=\psi_B \quad (5)$$

and

$$\text{(iii) } \frac{(\partial\psi_W/\partial z)}{m_w^*(E)}=\frac{(\partial\psi_B/\partial z)}{m_B^*(E)} \text{ for } |z|=L/2, \quad (6)$$

the well width is taken to be L, the subscripts W an B indicate the well and the barrier layer, and z is taken to be zero at the center of the well.

The confusion in the literature is about $m_i^*(E)$, the energy-dependent effective mass. It should be noted that $m_i^*(E)$ may be defined in the three following ways:

(i) Energy effective mass,

$$m_{ie}^*(E)=\hbar^2k_i^2/[2(E-E_{ci})]=m_i^*(0)[1+\alpha_i(E-E_{ci})], \quad (7)$$

(ii) Velocity (also called optic) effective mass,

$$m_{iv}^*(E)=\hbar^2k_i/\nabla_kE=m_i^*(0)[1+2\alpha_i(E-E_{ci})],$$

(iii) Acceleration effective mass,

$$m_{ia}^*(E)=\hbar^2/(\nabla_k)^2E\simeq m_i^*(0)[1+6\alpha_i(E-E_{ci})]. \quad (9)$$

All the three effective masses have been used in the literature, not only in the boundary condition but also for the evaluation of k_i from $(E-E_{ci})$. This is evidently a confusing situation and needs to be settled.

That energy effective mass is to be used for the determination of k_i from $(E-E_{ci})$, needs no further consideration, as this mass follows from the relation between k_i and $(E-E_{ci})$. On the other hand, the proper mass for the boundary condition is not clearly established, except that the acceleration effective mass has no relevance. Authors using the $\mathbf{k}\cdot\mathbf{p}$ perturbation method[21] for the analysis of nonparabolicity have concluded that the right mass is the energy effective mass. But, the energy effective mass does not ensure the continuance of current probability density. It has been argued[22] that this condition has no relevance as no current flows in the quantum well problem. On the

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other hand, for tunneling in barriers it has been argued[23] that the condition matches the phase velocity, and the requirement of group velocity is met when integration is carried out over different electron states for the evaluation of current density. These arguments justifying the applicability of energy effective mass in the boundary condition for the derivative are not acceptable as the boundary condition should not depend on the nature of the problem. In a single-barrier or double-barrier system, current flows through the system, and current due to an electron in the end contact layers is given by

$$J=(e/\hbar)\nabla_k E=e\hbar k/m^*(E);\ m^*(E)=m^*(0)(1+2\alpha E). \tag{10}$$

The continuity of current probability density, given by

$$J=\left(\frac{i\hbar}{m^*(E)}\right)\left(\psi^*\frac{\partial\psi}{\partial z}-\psi\frac{\partial\psi^*}{\partial z}\right), \tag{11}$$

is then ensured if $m^*(E)$ is replaced by the velocity effective mass. It is, therefore, the velocity effective mass which is the right mass for the boundary condition for $\partial\psi/\partial z$. This conclusion is in disagreement with that from the $\mathbf{k}\cdot\mathbf{p}$ theory and requires further examination of the $\mathbf{k}\cdot\mathbf{p}$ theory. It also appears that a final decision would depend on the evidence of experiments and for that we have to depend on more accurate experimental results than presently available.

We present in Fig. 1 the values of energy shifts calculated with the following constants for electrons:

$m^*_W=0.042m_0$; $m^*_B=0.079m_0$;

$\alpha_W=1.167(\text{eV})^{-1}$; $\alpha_B=0.83(\text{eV})^{-1}$

and for holes:

$m^*_W=0.47m_0$; $m^*_B=0.61m_0$; $\alpha_W=\alpha_B=0$;

m_0 is the free electron mass.

It was found that the results of earlier experiments were rather low and could not be fitted by using any reasonable value for $\Delta E_c/\Delta E_g$. These data are not shown in the figure. The results of more recent experiments shown in the figure may, however, be fitted mostly by taking $\Delta E_c/\Delta E_g=0.4$. It should be pointed out that the values of α, used in the present analysis, is consistent with that used generally in the analysis of transport experiments.

Sauer *et al.*[3] fitted the experimental data using a value of 0.63 for $\Delta E_c/\Delta E_g$ and a value of 3.3×10^{-19} m^2 for γ in the dispersion relation

$$E-E_c=(\hbar^2k^2/2m^*)(1-\gamma k^2).$$

This value for γ is equivalent to using for α, a value of $(2m^*/\hbar^2)\gamma=0.366$, which is far too low in comparison to the value used for the interpretation of transport experiments. This contradiction is really due to their use of the acceleration effective mass, which in effect underestimates the value of α. This is evident by considering the expressions for $m^*(E)$ given by (8) and (9). On using the value of α used in the present analysis, γ turns out to be 1.05×10^{-18} m^2, which is consistent with the value of

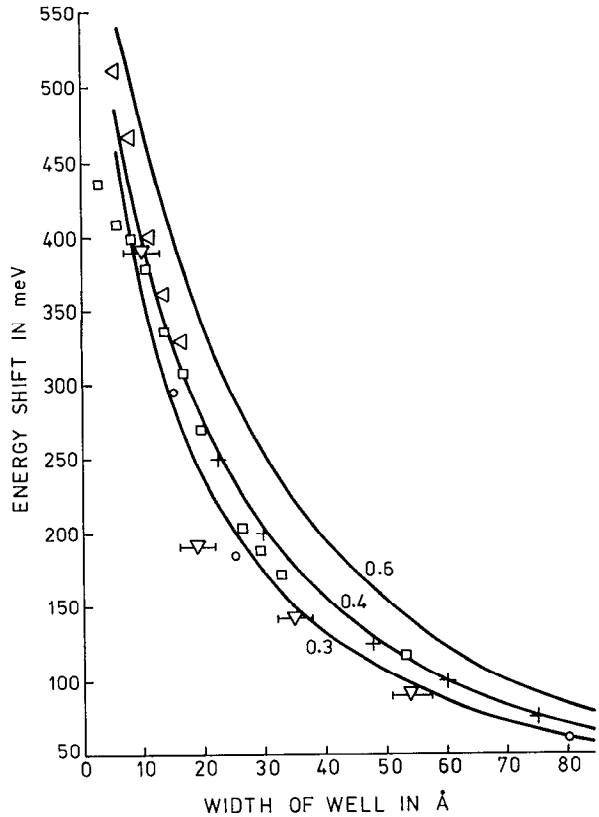

FIG. 1. Energy shift in InP/$Ga_{0.47}In_{0.53}As$ quantum wells. Numbers on the curves give the value of the ratio of the conduction-band discontinuity and the energy-gap discontinuity. (+) Sauer *et al.* (see Ref. 3), (∇) Carey *et al.* (see Ref. 15), (○) Morony *et al.* (see Ref. 12), (□) Seifert *et al.* (see Ref. 13), and ($\triangle$) Morais *et al.* (see Ref. 14).

3.3×10^{-19} m^2, obtained for GaAs,[24] as γ is expected to be inversely proportional to the product of effective mass m^* and energy-band gap, E_g.

It is also found that the value of α obtained for GaAs by analyzing the tunneling data[19] for single barriers with the energy effective mass in the boundary condition is 0.835 $(\text{eV})^{-1}$, which is higher than the value of 0.69 $(\text{eV})^{-1}$ obtained from the analysis of transport experiments.[25] Since the energy effective mass overestimates α in comparison to the velocity effective mass, this discrepancy is expected to be removed if the velocity effective mass is used in the boundary condition in the analysis of tunneling results.

In conclusion, it is found that the values of $\Delta E_c/\Delta E_g$ and α obtained for the InP/$Ga_{0.47}In_{0.53}As$ system from the analysis of photoluminescence data are consistent with other experimental values if the velocity effective mass is used in the boundary condition and the energy effective mass is used for obtaining k_i from $(E-E_{ci})$.

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