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In-plane effective mass in narrow quantum wells of nonparabolic semiconductors

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A formula is derived for the in-plane effective mass in narrow quantum wells, taking into account the effects of energy band nonparabolicity. The variation of the mass with the width of the well is studied by using the formula for four systems of wells. The mass is nearly the same as the velocity effective mass of the bulk material of the well in $GaAs/Ga_{0.7}Al_{0.3}As$ wells. It is about 8% larger in InAs/InP wells, but is significantly larger in very narrow wells of $Ga_{0.47}In_{0.53}As/InP$ systems. In the case of $InAs/Ga_{0.58}Al_{0.42}Sb$ wells, the in-plane mass differs from the well mass by large amounts for all well widths of interest.

The in-plane effective mass used for the evaluation of various electrical and optical transport coefficients is usually taken to be the same in a quantum well as in the bulk material constituting the well.[1,2] This assumption is applicable for widths of wells larger than about 10 nm. Much narrower wells, particularly of the strained layer[3,4] systems, are however, currently being studied for applications to devices. The in-plane mass may be significantly different[5,6] in narrow wells as the electron is not fully confined in such wells for finite barrier potentials. The electron stays part of the time in the barrier layer and as the effective mass is different in this layer, the effective value is determined by the occupation probabilities for the two layers. It may be shown[6] that for materials with parabolic energy bands the inverse of the effective value is the sum of the product of the inverse of the two masses and the corresponding occupation probabilities. However, as the energy eigenvalues are much higher in narrow wells the band nonparabolicity becomes significant, but no general formula is available for the in-plane mass of narrow wells of nonparabolic semiconductors.

The purpose of this letter is to derive a general formula for the in-plane effective mass for application to nonparabolic semiconductors, and to study the effective mass for different well widths in $GaAs/Ga_{0.7}Al_{0.3}As$, InAs/InP, $Ga_{0.47}In_{0.53}As/InP$, and $InAs/Ga_{0.58}Al_{0.42}Sb$ systems.

We consider a rectangular well of width L and barrier potential V_0. The z direction is chosen to be perpendicular to the plane of the well, with $z=0$ at the center. The equation for the envelope function,[7] $F_i(z,\rho)$ may be written as:

$$[\hbar^2/2m_{Ei}(E_T)]\nabla^2 F_i(z,\rho)+(E_T-E_{ci})F_i(z,\rho)=0, \tag{1}$$

where E_{ci} represents the band-edge energy, E_T is the energy eigenvalue including the component due to the in-plane motion, ρ is the in-plane position coordinate; $m_{Ei}(E)$ is the energy effective mass[8] of the bulk material constituting the i layer. The ratio of the square of the crystal momentum, $\hbar k$, and two times this mass gives the electron energy, E-E_{ci}. The index i should be replaced by W for the well layer and by B for the barrier layer.

The envelope function may be expressed for an electron with the in-plane wave vector k_i as

$$F_i(z,\rho)=\phi_i(z)\exp(i\mathbf{k}_i\rho), \tag{2}$$

where $\phi_i(z)$ is the z-dependent part of $F_i(z,\rho)$. Equation (1) is solved by using the boundary conditions:

$$F_B(\pm\infty,\rho)=0, \quad F_B(\pm L/2,\rho)=F_W(\pm L/2,\rho), \tag{3}$$

$$(1/m_{vB})(\partial F_B/\partial z)_{z=\pm L/2}=(1/m_{vW})(\partial F_W/\partial z)_{z=\pm L/2}, \tag{4}$$

where m_{vi} is the velocity effective mass,[9–11] of the bulk material of the i layer. The ratio of the crystal momentum and this mass gives the electron velocity $\hbar^{-1}\nabla_k E$.

Condition (3) gives $k_B=k_W$. Putting $k_B=k_W=k_t$, we get

$$[\hbar^2/2m_{Ei}(E_T)]\partial^2\phi_i/\partial z^2+[(E_T-E_{ci}) -\hbar^2 k_t^2/2m_{Ei}(E_T)]\phi_i=0. \tag{5}$$

It may be easily shown that the energy eigenvalue is given for the ground state by the equation:

$$\tan k_{zW}L/2=k_{zB}m_{vW}/k_{zW}m_{vB}, \tag{6}$$

where k_{zW} and k_{zB} are, respectively, the wave vector and decay constant in the well and the barrier, for motion along the z-direction. These are given by

$$k_{zW}^2=(2m_W/\hbar^2)\gamma_W(E_0)-k_t^2;$$
$$k_{zB}^2=(2m_B/\hbar^2)[-\gamma_B(E_0-V_0)]+k_t^2. \tag{7}$$

$$E_0=E_T-E_{cW}; \; V_0=E_{cB}-E_{cW}. \tag{8}$$

The nonparabolic dispersion relation has been assumed to be the same as the simplified Kane relation[9–13] for the bulk materials given below:

$$(\hbar^2 k^2/2m_i)=E(1+\alpha_i E)=\gamma_i(E), \tag{9}$$

where m_i is the band-edge-effective mass for the bulk material, E is the energy of the electron measured from the band edge, $\mathbf{k}$ is the three-dimensional wave vector and α_i is the nonparabolicity parameter, given approximately by[13]

$$\alpha_i=(1-m_i/m_0)^2(1/E_g^*). \tag{10}$$

E_g^* is the effective energy band gap, often smaller than the actual band gap, E_g, and m_0 is the free-electron mass.

It may be noted that the energy and the velocity effective masses are given for this nonparabolic relation by,

$$m_{Ei}(E_T)=m_i\gamma_i(E_T-E_{ci})/(E_T-E_{ci});\ m_{vi}(E_T)$$
$$=m_i(\partial/\partial E_T)[\gamma_i(E_T-E_{ci})]\ . \qquad (11)$$

The eigenvalues of energy, E_0, may be expressed as,

$$E_0=E_e(V,k_t^2)+\hbar^2k_t^2/2m_{EW}(E_0);$$
$$V=V_0-(\hbar^2k_t^2/2)[1/m_{EW}(E_0)-1/m_{EB}(E_0)]\ . \qquad (12)$$

$E_e(V,k_t^2)$ is the component of energy corresponding to the quantized z component of the wave vector. It is seen that the effective barrier potential V and hence E_0 depends on k_t^2.

It may be shown by using Eq. (12) that the in-plane effective mass, m^*, which is given by $\hbar^2k_t[(\partial E_0/\partial k_t)_{k_t\to 0}]^{-1}$ may be expressed as

$$1/m^*=[1/m_{EW}(E_0)-(\partial E_e/\partial V)_{k\to 0}(1/m_{EW}(E_0)$$
$$-1/m_{EB}(E_0)][1-(\partial E_e/\partial E_t)_{k_t\to 0}]^{-1}\ . \qquad (13)$$

It may be mentioned that the three masses, m_{Ei}, m_{vi}, and m_i, defined earlier, are for the bulk material of the well or the barrier. These have the same value for parabolic E-k relation, but are different for finite values of E in nonparabolic materials. The in-plane effective mass, given by Eq. (13), on the other hand, determines for a quantum well its in-plane transport properties, e.g., cyclotron resonance frequency, mobility, and intersubband optical absorption. It is characteristic of a particular well and is determined by both the well and the barrier layer and by the dimensions of the well.

The term $(\partial E_e/\partial V)_{k_t\to 0}$ is equal to θ, the occupation probability for the barrier layers,[6] An expression for $(\partial E_e/\partial E_T)_{k_t\to 0}$ as given below may also be obtained by differentiating Eq. (6)

$$(\partial E_e/\partial E_T)_{k_t\to 0}=\{E_0(E_0-V_0)\alpha_B/\gamma_B(E_0-V_0)-4E_0\alpha_B/(\partial/\partial E_0)[\gamma_B(E_0-V_0)]+4E_0\alpha_W/(\partial/\partial E_0)[\gamma_W(E_0)]$$
$$-[E_0^2\alpha_W/\gamma_W(E_0)][1+k_{zW}L/\sin(k_{zW}L)]\}[1+k_{zW}L/\sin(k_{zW}L)+E_0/(V_0-E_0)]^{-1}\ . \qquad (14)$$

Equation (13) then gives the in-plane effective mass with $(\partial E_e/\partial V)_{k_t\to 0}=\theta$ and $(\partial E_e/\partial E_T)_{k_t\to 0}$ given by Eq. (14).

In-plane effective mass was studied by using (13) for the ground state in the four systems: $GaAs/Ga_{0.7}Al_{0.3}As$, InAs/InP, $Ga_{0.47}In_{0.53}As/InP$, and $InAs/Ga_{0.58}Al_{0.42}Sb$. The physical constants used in the calculations are given in Table I. It should be noted that the nonparabolicity parameter for GaAs and InP were obtained from **k**·**p** calculations using five or more bands and the values of E_g^* were found to be significantly lower than E_g. Such values are not, however, available for the other materials and the required values of α_i were obtained by using Eq. (10) and the actual band gap, E_g, for E_g^*.

TABLE I. Physical constants for quantum wells. The band-edge effective mass for the well, m_w^*, and for the barrier, m_B^*, are in units of m_0; the corresponding nonparabolicity parameters α_W and α_B are in units of $(eV)^{-1}$ and the barrier height V_0 is in units of meV.

Material	m_W^*	m_B^*	α_W	α_B	V_0
$Ga_{0.47}In_{0.53}As/InP$	0.042[a]	0.079[a]	1.09[b]	0.83[c]	240[d]
$GaAs/Ga_{0.7}Al_{0.3}As$	0.0665[e]	0.095[e]	0.885[f]	0.631[f]	261[e]
$InAs/Ga_{0.58}Al_{0.42}Sb$	0.0239[a]	0.089[a]	2.04[b]	0.68[b]	1140[g]
InAs/InP	0.0239[a]	0.079[a]	2.04[b]	0.83[c]	500[h]

[a]*Semiconductors*, edited by O. Madelung (Springer, Berlin, 1991), pp. 126, 134, 152, and 154.
[b]Calculated by using the values of the band gap and spin-orbit splitting.
[c]K. Brennan and K. Hess, Solid-State Electron. 27, 347 (1984).
[d]B. R. Nag and S. Mukhopadhyay, Appl. Phys. Lett. 58, 1056 (1991).
[e]D. F. Nelson, R. C. Miller, and D. A. Kleinmann, Phys. Rev. B 35, 7770 (1987).
[f]Calculated by using the value of γ.
[g]R. Beresford, L. F. Luo, and W. I. Wang, Appl. Phys. Lett. 54, 1899 (1989).
[h]This value gives the best fit to the data of Ref. 4, when band nonparabolicity is taken into account.

Calculated values of m^* are presented in Fig. 1 for the $GaAs/Ga_{0.7}Al_{0.3}As$ and $Ga_{0.47}In_{0.53}As/InP$ system and in Fig. 2 for the InAs/InP and $InAs/Ga_{0.58}Al_{0.42}Sb$ systems. It should be mentioned that calculations were also done by the exact method, in which Eq. (6) is solved for different values of k_t and then m^* is obtained from the derivative $(\partial E_0/\partial k_t)$. The results of exact calculations were the same as those obtained from (13), and hence these are not separately shown. Values of the velocity effective mass for the bulk well material corresponding to E_0, are, however, given in the figures to indicate the change in the values caused by wave function penetration.

It is seen from Fig. 1 that the wave function penetration increases the effective mass by about 8% for the strained layer InAs/InP system for all widths smaller than 8 nm. In the case of $Ga_{0.47}In_{0.53}As/InP$ the effect is still larger. The difference increases to about 15.5% for a well width of 1 nm. Values for the $GaAs/Ga_{0.7}Al_{0.3}As$ system, however, lies within 2% of the bulk value and is, in fact, slightly higher for very narrow wells. This result may be understood by considering that the mass of the bulk material of the well and the barrier layer are nearly the same in this system when the effect of nonparabolicity is taken into account and also that the well mass is a little higher

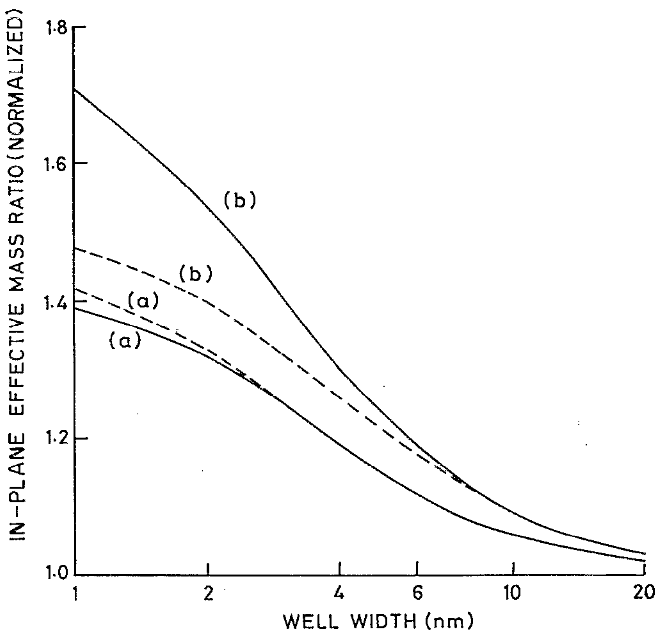

FIG. 1. In-plane effective mass ratio for different well widths, normalized by the band-edge effective mass ratio for the bulk well material. (a) $GaAs/Ga_{0.7}Al_{0.3}As$ system. (b) $Ga_{0.47}In_{0.53}As/InP$ system. Solid line: In-plane effective mass of the quantum well system. Dashed line: Velocity effective mass of the bulk well material for the subband energy.

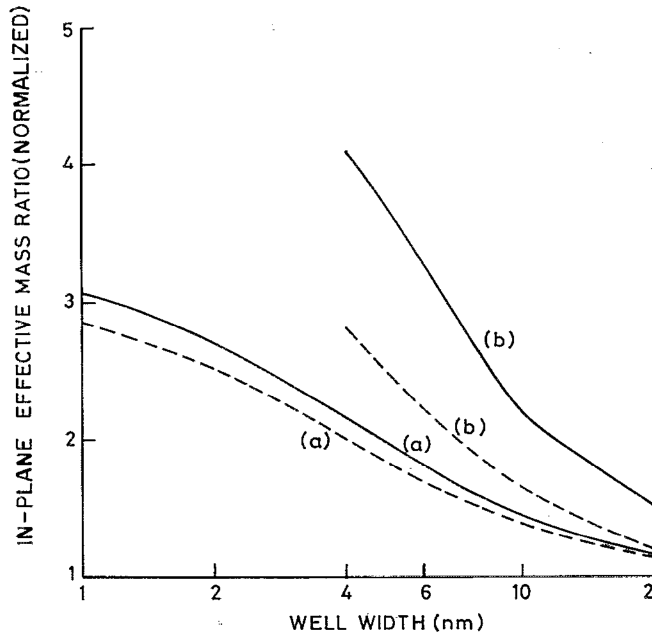

FIG. 2. In-plane effective mass ratio for different well widths, normalized by the band-edge effective mass ratio for the bulk well material. (a) InAs/InP system. (b) $InAs/Ga_{0.58}Al_{0.42}Sb$ system. Solid line: In-plane effective mass of the quantum well system. Dashed line: Velocity effective mass of the bulk well material for the subband energy.

than the barrier mass for the energy eigenvalues of narrow wells.

Values are given for the $InAs/Ga_{0.58}Al_{0.42}Sb$ system for well widths down to 4 nm only, corresponding to which the energy eigenvalue is 440 meV. The nonparabolic relation used in the calculation would not be valid for higher energies and hence the computed value would have no relevance. It is, however, seen that the in-plane mass for this system differ from the well mass by 25% even for a well width of 20 nm. The difference increases to 50% for a well width of 4 nm.

It should be mentioned that, although we have included the nonparabolicity of the barrier layer, its effect may be considered relatively unimportant. This is because the energy eigenvalue is close to the band edge of the barrier layer for wells in which the wave function penetration is significant.

In summary, a formula has been derived for the calculation of in-plane effective mass in narrow quantum wells of nonparabolic semiconductors. The formula gives results identical with those obtained from the exact method. It is also found that the in-plane effective mass is not significantly altered from the velocity effective mass of the bulk material of the well in $GaAs/Ga_{0.7}Al_{0.3}As$ systems. Alterations are, however, large in InAs/InP and still larger in the $Ga_{0.47}In_{0.53}As/InP$ system for very narrow wells. On the other hand, values are largely altered in $InAs/Ga_{0.58}Al_{0.42}Sb$ systems even for fairly large well widths.

The results cannot be compared with experiments at present, as no measurement of the in-plane effective mass of narrow wells has been reported. The calculations reported in this letter, however, indicate that the in-plane effective mass of narrow wells would be determined by the band nonparabolicity of the well material and also by the barrier layer mass. Measurement of the in-plane effective mass would, therefore, be useful for studying these parameters.

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