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Deformation potential acoustic phonon scattering limited mobility in narrow quantum wells

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Abstract. The form factor and the effective mass are shown to be significantly altered in narrow quantum wells owing to the extension of the wavefunction into the barrier layers. The mobility is found to change as a result by a large factor (a factor of 12 for a well width of 0.5 nm). Modifications caused by the band non-parabolicity are also discussed.

1. Introduction

The technology of growth of quantum well systems has been so refined that quantum wells may be realized with a thickness of few monolayers (Uomi *et al* 1990, Wang *et al* 1990). The wavefunction of the confined electrons enters deeply into the barrier layers in such systems. This penetration is likely to affect the transport of electrons in planes parallel to the interface as the electron spends part of the time in the barrier layer. However, the electron mobility has been discussed in the literature for heterostructures and quantum wells without considering the effect of the penetration. The discussion has been confined to wells of widths larger than 5 nm. The wavefunction penetration is not expected to be large in such wells. Hence the effect has not received much attention except as a passing reference (Ando 1982). The purpose of this paper is to derive the relevant formulae and to assess the effect of this extension on electron mobility limited by deformation potential acoustic phonon scattering, which is the dominant scattering mechanism near the liquid-nitrogen temperature (Ridley 1982, Walukiewicz *et al* 1984).

2. Equivalent effective mass

A rectangular potential well extending from $z = -L/2$ to $z = L/2$ is considered. The wavefunction is obtained by solving the Schrödinger equation with the effective-mass formalism. The equation is

$$(\hbar^2/2m_i^*)\nabla^2\psi_i + (E - E_{ci})[1 + \alpha_i(E - E_{ci})]\psi_i = 0 \qquad (1)$$

where m_i^* is the band edge effective mass, E is the total energy and E_{ci} is the band edge energy. A non-parabolic band is assumed, which obeys the Kane E–k dispersion relation (Nag 1980)

$$\hbar^2k^2/2m_i^* = (E - E_{ci})[1 + \alpha_i(E - E_{ci})] \tag{2}$$

the non-parabolicity parameter α_i being given by (Nelson *et al* 1987)

$$\alpha_i = (E_{gi} + \Delta_i/3)^{-1} \tag{3}$$

where E_{gi} is the direct energy band gap and Δ_i is the spin–orbit splitting. The subscript i is replaced by W for the well layer and by B for the barrier layer. The non-parabolic band is considered as the confinement energy is large in narrow wells and non-parabolicity may have a significant contribution. Solution of (1) is sought in the form

$$\psi_i = F_i(z)\exp(-\mathrm{i}\boldsymbol{k}_{\perp i}\cdot\boldsymbol{\rho}) \tag{4}$$

where $\boldsymbol{\rho}$ is a position vector in planes parallel to the interface, $\boldsymbol{k}_{\perp i}$ is the corresponding wavevector and $F_i(z)$ is the envelope function. The boundary conditions for ψ at the interfaces are

$$\psi_W = \psi_B \tag{5}$$

and

$$[1/m_W^*(E)](\mathrm{d}\psi_W/\mathrm{d}z) = [1/m_B^*(E)](\mathrm{d}\psi_B/\mathrm{d}z) \tag{6}$$

where $m_i^*(E)$ is required to be evaluated using (2). There has been some controversy about the exact expression for $m_i^*(E)$. It has been concluded from the $\boldsymbol{k}\cdot\mathbf{p}$ perturbation analysis that it should be the energy effective mass given by (Bastard 1982)

$$m_\varepsilon^*(E) = \hbar^2k^2/2(E - E_{ci}). \tag{7}$$

On the other hand, it has been pointed out that this effective mass does not ensure continuation of the current probability density across the interface, which may, however, be ensured by using the velocity effective mass, given by

$$m_v^*(E) = \hbar^2k/\nabla_k E. \tag{8}$$

We have used the energy effective mass, as this formulation has current acceptance.

The boundry condition (6) implies that

$$k_{\perp W} = k_{\perp B} \tag{9}$$

and

$$F_W(z) = F_B(z). \tag{10}$$

Also,

$$[1/m_W^*(E)][\mathrm{d}F_W(z)/\mathrm{d}z] = [1/m_B^*(E)][\mathrm{d}F_B(z)/\mathrm{d}z]. \tag{11}$$

The envelope function $F_i(z)$ is the solution of the equation

$$(\hbar^2/2m_i)[\mathrm{d}^2F_i(z)/\mathrm{d}z^2] + (E - E_{ci})[1 + \alpha_i(E - E_{ci})]F_i(z) - (\hbar^2k_{\perp i}^2/2m_i^*)F_i(z) = 0. \tag{12}$$

It is easily appreciated that the energy eigenvalues corresponding to the longitudinal component of momentum depend on the transverse component of the wavevector for non-parabolic bands. A further dependence is found to occur when m_W^* and m_B^* are not

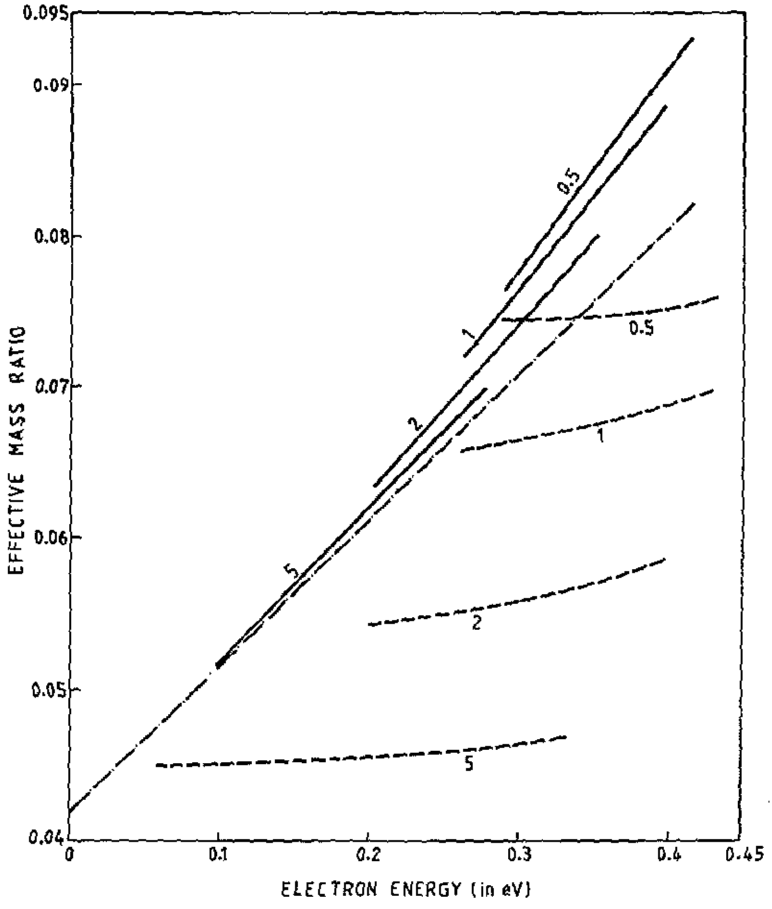

Figure 1. Effective mass ratio for different electron energies: – – –, parabolic band; ———, non-parabolic band; – · –, non-parabolic band neglecting wave penetration into the barriers. The numbers on the curves give the widths of the wells in nanometres.

equal and the conservation of transverse momentum is taken into account. This latter effect may be made evident by considering a parabolic band and writing

$$E - E_{cW} - \hbar^2 k_\perp^2/2m_W^* = E' \tag{13}$$

$$k_{\perp W} = k_{\perp B} = k_\perp . \tag{14}$$

The equation then takes the form

$$(\hbar^2/2m_i^*)[d^2F_i(z)/dz^2] + [E' - V_i(k_\perp)]F_i(z) = 0 \tag{15}$$

and

$$V_W(k_\perp) = 0 \tag{16}$$

$$V_B(k_\perp) = E_{cB} - E_{cW} - \Delta V_B \tag{17}$$

$$\Delta V_B = (\hbar^2 k_\perp^2/2)(1/m_W^* - 1/m_B^*). \tag{18}$$

Thus, the barrier potential is reduced effectively by ΔV_B, which is proportional to

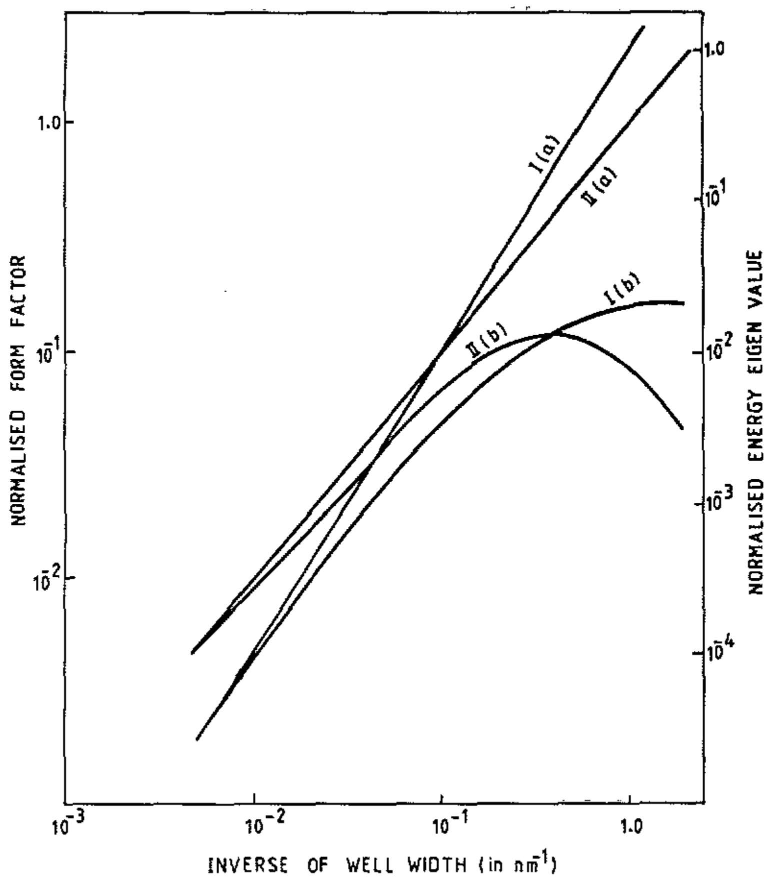

Figure 2. Energy eigenvalues (curves I) and form factors (curves II) normalized by their values for a 1 nm well with an infinite barrier height: curves (a), infinite barrier height; curves (b), finite barrier height.

$k_\perp^2$. This change in V_B causes the energy eigenvalue E' corresponding to the longitudinal component of momentum to vary with the transverse component of the wavevector. This dependence effectively alters the effective mass corresponding to the itinerant energy even when non-parabolicity is neglected.

The altered masses m_v^* and m_e^* may be obtained by considering that the itinerant energy

$$E_I = E(k_\perp) - E(0) = \hbar^2 k_\perp^2/2m_e^* \tag{19}$$

$$= E'(k_\perp) - E'(0) + \hbar^2 k_\perp^2/2m_W^*. \tag{20}$$

m_v^* and m_e^* are hence given by

$$1/m_v^*(E_I) = (1/\hbar^2 k_\perp)(\partial E_I/\partial k_\perp) = 1/m_W^* + (1/\hbar^2 k_\perp)(\partial E'/\partial k_\perp) \tag{21}$$

$$1/m_e^*(E_I) = 2E_I/\hbar^2 k_\perp^2 = 1/m_W^* + 2[E'(k_\perp) - E'(0)]/\hbar^2 k_\perp^2. \tag{22}$$

We illustrate in figure 1 the variation in the velocity effective mass m_v^* with E and well width for the $InP/Ga_{0.47}In_{0.53}As/InP$ system. The physical constants were taken

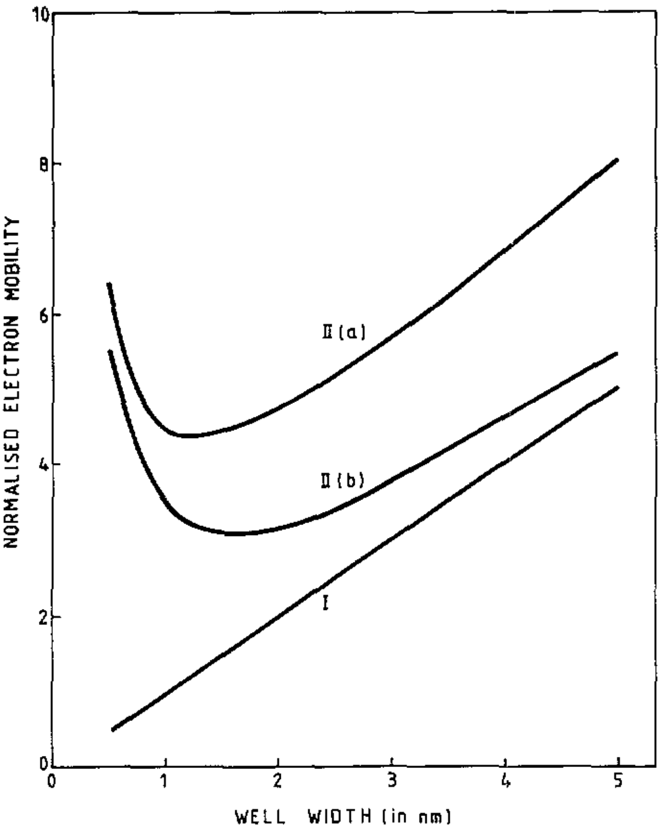

Figure 3. Electron mobility for different widths normalized by its value for a 1 nm well with infinite barrier height: line I, infinite barrier height; curve IIa, finite barrier height, parabolic band; curve IIb, finite barrier height, non-parabolic band.

as follows: $m^*_W = 0.042m_0$; $\alpha_W = 1.167\,\text{eV}^{-1}$; $m^*_B = 0.078m_0$; $\alpha_B = 0.83\,\text{eV}^{-1}$; $E_{cB} - E_{cW} = 300\,\text{meV}$; $m_0 = 9.1 \times 10^{-31}\,\text{kg}$.

It is seen that the effective mass m^*_v increases asymptotically from the value of $0.042m_0$ for wide wells to $0.078m_0$ for narrow wells. The increase in effective mass is partly due to non-parabolicity and partly due to the penetration of the wavefunction. The individual contributions and the total effect are illustrated in figure 1. The energy effective mass m^*_e is not illustrated. Its variation is similar, but the magnitude is smaller.

3. Scattering probability and mobility

The extension of the wavefunction into the barrier layer alters the scattering probability by changing the effective mass and, in addition, the form factor. Only the deformation potential acoustic phonon scattering is considered to illustrate the effect, keeping the computations simple. The scattering probability is given by (Ridley 1982)

$$S(k_\perp) = c_{\rm ac}[m_{\rm v}^*(E_{\rm I})/m_{\rm v}^*(0)]I \tag{23}$$

where

$$c_{\rm ac} = E_1^2 k_{\rm B} T m_{\rm v}^*(0)/4\pi\rho s^2 \hbar^3$$

$$I = \int_{-\infty}^{\infty} |G(q_z)|^2 \,{\rm d}q_z$$

$$G(q_z) = \int_{-\infty}^{\infty} \psi^*\psi \cos(q_z z)\,{\rm d}z$$

$$\psi = H(|z| - L/2)\psi_{\rm B} + H(L/2 - |z|)\psi_{\rm W}.$$

$H(x)$ is the Heaviside function and other symbols have their usual meanings. In the theories of scattering reported in the literature, $G(q_z)$ is usually evaluated by assuming that the well is of infinite depth, so that $\psi_{\rm B}$ may be taken to be zero. The integral I in (23) then has a value of $3\pi/L$ (L is the width of the well). The value obtained by using the solutions for finite barriers is shown in figure 2, which illustrates the effect of penetration. It should be mentioned that the energy corresponding to the transverse momentum has been neglected in this calculation as it is a small fraction of the total energy which determines the penetration. The effect of non-parabolicity is also made evident by presenting the results for a parabolic band. It is seen that the penetration has the general effect of reducing the form factor, which reduces the scattering probability. This reduction is, however, partially cancelled by the increase in the equivalent effective mass. However, the overall effect is a reduction in scattering, which enhances the mobility from the infinite-well value.

The mobility μ may be calculated using the above results with the formula

$$\mu = [|e| m_{\rm v}^*(0)/c_{\rm ac} I k_{\rm B} T]\left[\int_0^\infty \frac{m_{\rm e}^*(E_{\rm I})}{m_{\rm v}^*(E_{\rm I})^2}\exp\left(-\frac{E_{\rm I}}{k_{\rm B}T}\right) E_{\rm I}\,{\rm d}E_{\rm I}\right] \times \left[\int_0^\infty m_{\rm v}^*(E_{\rm I})\exp\left(-\frac{E_{\rm I}}{k_{\rm B}T}\right){\rm d}E_{\rm I}\right]^{-1}. \tag{24}$$

Further, for narrow wells, only one confined energy level needs to be considered as either one such level exists or the separation of the second level is much larger than the thermal energy.

We present in figure 3 the mobility normalized by its value for the infinite-barrier well with a width of 1 nm. The results may be explained from the following considerations. The mobility limited by deformation potential acoustic phonon scattering varies directly as the width of the well in the infinite-barrier approximation. This result may be explained by considering that the scattering probability due to the deformation potential acoustic phonons in bulk interactions varies as the square root of the electron energy. As the confined energy in the infinite-barrier approximation is proportional to the inverse of the square of the well width, and the itinerant energy is small in comparison with the confinement energy, the scattering probability for the confined electron varies as the inverse of the width and hence the mobility varies directly as the width. For finite barriers, the confined energy is not proportional to the inverse square of the well width and is much lower than given by the infinite-barrier model (see figure 2). This lowering causes an increase in the mobility. The actual values of mobility are, however, somewhat lowered from this increased value by the penetration of the wavefunction in the barrier layer, which causes an increase in the effective mass.

4. Conclusion

A theory of electron mobility has been presented for narrow quantum wells with finite-barrier potentials. Detailed results have been worked out for deformation potential acoustic phonon scattering including the effects of energy band non-parabolicity. Numerical values are given for the $InP/Ga_{0.47}In_{0.53}As/InP$ system. It is found that the mobility is much larger than that given by the infinite-barrier-potential approximation and the ratio of the calculated mobility to its approximate value increases from a factor of 1.4 for a 10 nm well to 12 for a 0.5 nm well.

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