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SELF–CONSISTENT CALCULATIONS OF CHARGE TRANSFER AND ALLOY SCATTERING-LIMITED MOBILITY IN InP-$Ga_{1-x}In_xAs_yP_{1-y}$ SINGLE QUANTUM WELLS

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We present the results of self-consistent calculations of charge transfer and alloy scattering-limited mobility in modulation-doped InP-$Ga_{1-x}In_xAs_yP_{1-y}$ single Quantum Wells at $T = 0$. The band-bending is treated in perturbation and the Electric Quantum Limit is assumed. Ternary Quantum Wells ($y = 1$) are calculated to have a lower mobility than single InP-$Ga_{1-x}In_x$As heterojunctions, all material parameters being the same in both kinds of structures.

THE SEMICONDUCTOR quantum wells (Q.W.) consisting of $Ga_{1-x}In_x$As or $Ga_{1-x}In_xAs_yP_{1-y}$ latticed-matched to InP barriers appear promising for optoelectronics since their effective band gap can be adjusted to fit the photon energy range where the optical fibers display minimal losses. Compared with GaAs-$Ga_{1-x}Al_x$As Q.W.'s the ternary or quaternary-based Q.W.'s should display a stronger alloy scattering. The latter mechanism has recently been shown [1, 2] to be dominant in InP-$Ga_{1-x}In_x$As single heterojunctions at low temperatures. Here we report the results of calculations of the energy levels and alloy scattering-limited mobility in modulation doped $Ga_{1-x}In_x$As-InP, $Ga_{1-x}In_xAs_yP_{1-y}$-InP single quantum well structures.

In contrast with single heterostructures the band bending arising from charge transfer from InP to the ternary or quaternary material can be treated in perturbation which makes the calculates easier. Also the short-range nature of the alloy scattering potential allows simplifications in the treatment of transport equations. Noticeably the mobility drop which takes place when an excited electronic subband becomes populated is analytically obtained. Our calculations show that a typical $Ga_{1-x}In_x$As-InP quantum well (thickness $L = 100$ Å, $2D$ electron concentration $n_e = 4 \times 10^{11}$ cm^{-2}) should have a lower alloy scattering-limited mobility ($\sim 5 \times 10^4$ cm^2 Vs^{-1}) than the one displayed by a single InP-$Ga_{1-x}In_x$As heterojunction with the same n_e ($\sim 2 \times 10^5$ cm^2 Vs^{-1}). Quaternary quantum wells should have an even lower mobility, although exact figures can be hardly obtained due to the lack of knowledge of several parameters.

We consider a single InP-$Ga_{1-x}In_xAs_yP_{1-y}$ Q.W. of thickness L. In this system InP is the barrier and the alloy is the well. The conduction band discontinuity will be denoted by V_b. The static dielectric constant ϵ will be taken as a constant over the whole structure: $\epsilon = \sqrt{\epsilon_{InP}\epsilon_{alloy}}$ where $\epsilon_{InP} = 12.4$ and $\epsilon_{alloy} = 14$ for $Ga_{0.47}In_{0.53}$As. The quaternary alloy is assumed to be lattice-matched to InP which implies:

$$(1-x)(1.032-0.032y) = 0.47y. \tag{1}$$

Finally we assume that InP contains a net volume concentration of N_d donors per cubic centimeter. The residual doping ($\lesssim 10^{16}$ cm^{-3}) of the alloy plays a negligeable part in the charge transfer mechanism and will be neglected hereafter. Note, however, that it will contribute to the mobility limited by Coulombic scattering. In the Electric-Quantum Limit (E.Q.L.) and in the Hartree approximation we have to solve self-consistently

$$\phi''(z) = \frac{4\pi e}{\epsilon}\{n_e\psi_1^2(z) - N_d Y(z^2 - L^2/4)\} \tag{2}$$

$$\left\{-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} - e\phi(z) + V_b Y(z^2 - L^2/4)\right\}\psi_1(z) = E_1\psi_1(z), \tag{3}$$

where $Y(x)$ is the step function ($Y(x) = 1$ if $x > 0$, $Y(x) = 0$ if $x < 0$) and m^* is the carrier effective mass which we take constant throughout the whole structure.

A significant difference between modulation-doped quantum wells (M.D.Q.W.) and single heterojunction (H.J.) lies in the smaller influence of ϕ on the energy levels in Q.W. Even if ϕ is zero E_1 is bound in Q.W.'s whereas under the same condition a single H.J. does not exhibit any bound state. Thus if n_e is not too large we may treat ϕ as a perturbation of the unperturbed (i.e. $\phi = 0$) Q.W. energy levels. Such procedure has already been successfully used by Fishman [3] in the

case of modulation-doped GaAs-$Ga_{1-x}Al_xAs$ Q.W.'s Fishman [3] diagonalized ϕ between three or four Q.W. bound levels. Here we use a reduced version of Fishman's approach. Namely we consider only the first order energy shifts of E_1. This is motivated by the fact that, for the symmetric structures under consideration, ϕ does not couple E_1 with E_2 (since those two states have opposite parities) but with $E_3, E_5 \ldots$ These levels may often not exist in InP-$Ga_{1-x}In_xAs_yP_{1-y}$ due to the light conduction mass of the alloys and the Q.W. thickness of our interest: $L \lesssim 200$ Å. In this first-order approach equations (2, 3) decouple. The solution of equation (2) is given by:

$$E_1 = E_1^{(0)} + \langle \psi_1^{(0)} | -e\phi | \psi_1^{(0)} \rangle \tag{4}$$

$$\psi_1(z) = \psi_1^{(0)}(z) = \begin{cases} A \cos k_w z & |z| \leqslant L/2 \\ B \exp\left[-k_b(z - L/2)\right] & z > L/2 \\ B \exp\left[k_b(z + L2)\right] & z < -L/2 \end{cases} \tag{5}$$

where $\psi_1^{(0)}$ is the unperturbed Q.W. ground state wavefunction,

$$\frac{\hbar^2 k_w^2}{2m^*} = E_1^{(0)} = V_b - \frac{\hbar^2 k_b^2}{2m^*} \tag{6}$$

and A and B are determined by the boundary and normalization conditions. The potential $\phi(z)$ is obtained by integrating equation (2) twice with $\psi_1(z)$ replaced by $\psi_1^{(0)}(z)$ with the boundary conditions that ϕ and ϕ' are continuous at $z = \pm L/2$ and by requiring that the electric field vanishes at the end of the donor depletion length in the barrier L_d. At $T = 0$ the equilibrium conditions for the structure are

$$E_1 + \frac{\pi\hbar^2 n_e}{m^*} = V_b - R_b - \frac{2\pi e^2}{\epsilon} N_d L_d^2 \tag{7}$$

$$2N_d L_d = n_e, \tag{8}$$

where R_b is the donor binding energy in the barrier which if the donor is hydrogenic is quite small (~ 6 meV). In equation (7) the potential drop associated with the penetration of the electron wavefunction in the barrier has been neglected. We show in Fig. 2 the calculated transferred charge in InP-$Ga_{0.47}In_{0.53}As$ modulation-doped Q.W.'s versus the well thickness L. The barrier doping has been taken constant: $N_d = 3 \times 10^{16}$ cm^{-3} which corresponds to a plausible residual doping in InP [4, 8]. Since V_b is not very well known in InP-$Ga_{0.47}In_{0.53}As$ the calculations have been performed for three values of $V_b - R_b$: 0.2 eV, 0.35 eV, 0.5 eV. We notice in Fig. 2 a decrease of the transferred charge in narrow wells. It is due to the increased

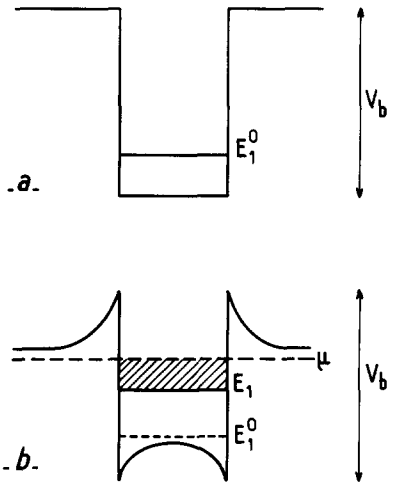

Fig. 1. Conduction-band profile of a modulation-doped n-type semiconductor quantum well.

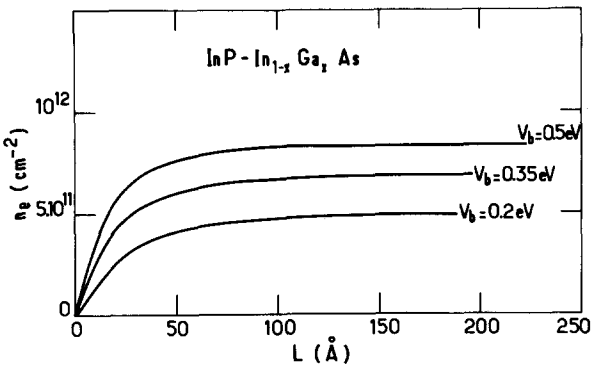

Fig. 2. Two-dimensional electron concentration versus well thickness in modulation-doped single InP-$In_{0.53}Ga_{0.47}As$ quantum well. Three values of V_b are considered (V_b = 0.2 eV, 0.35 eV and 0.5 eV).

confinement energy $E_1^{(0)}$ ($E_1^{(0)} \to V_b$ when $L \to 0$). It may also be remarked in Fig. 2 that the transferred charge changes very little once $L \gtrsim 100$ Å. This behaviour reflects the smaller part played by E_1^0 in equation (7). In Fig. 2 the curves have been interrupted when the second level E_2 becomes populated since then the equations (2–8) are no longer self-consistent.

To calculate the mobility limited by alloy scattering at $T = 0$ we consider the coupled system linking the velocity relaxation times $\tau_i(E_F)$ of the ith occupied subband to the Fermi energy E_F [5]:

$$E_F - E_i = \sum_j K_{ij}\tau_j(E_F). \tag{9}$$

In the E.Q.L. only K_{11} is different from zero. To evaluate the alloy scattering contribution to K_{11} (E_F) we consider the ternary alloy in the virtual crystal approximation (V.C.A.) at the zero th order and treat

the difference between the random alloy potential and the virtual crystal potential in the Born approximation. We thus obtain the alloy scattering limited mobility as

$$\mu_{\text{alloy}}(E_F) = \frac{e\hbar^3}{(m^*)^2\Omega_0 x(1-x)[\delta V]^2} \times \times \frac{1}{\int_{L/2}^{L/2} |\psi_1(z)|^4 \, dz}, \quad (10)$$

where Ω_0 is the volume of the V.C.A. unit cell; $[\delta V]$ the strength of the fluctuating alloy potential averaged over Ω_0 and $x = 0.53$ for $Ga_{0.47}In_{0.53}As$. When the second subband has just become populated ($E_F = E_2$) intersubband scattering becomes operative. The short-range nature of the alloy scattering allows to obtain a simple expression for the relative mobility variation at the onset of the intersubband scattering:

$$\frac{\Delta\mu}{\mu} = \frac{\mu(E_F = E_2^+) - \mu(E_F = E_2^-)}{\mu(E_F = E_2^-)} = \frac{-\int_{-L/2}^{L/2} [\psi_1(z)]^2 [\psi_2(z)]^2 \, dz}{\int_{-L/2}^{+L/2} [\psi_1(z)]^2 [[\psi_1(z)]^2 + [\psi_2(z)]^2] \, dz} \quad (11)$$

where $\psi_2(z)$ is the E_2 state wavefunction. The Fig. 3 presents the L dependence of the mobility limited by alloy scattering in InP-$Ga_{0.47}In_{0.53}As$ Q.W. for three different values of the conduction band offset V_b. Several features are noticeable in Fig. 3.

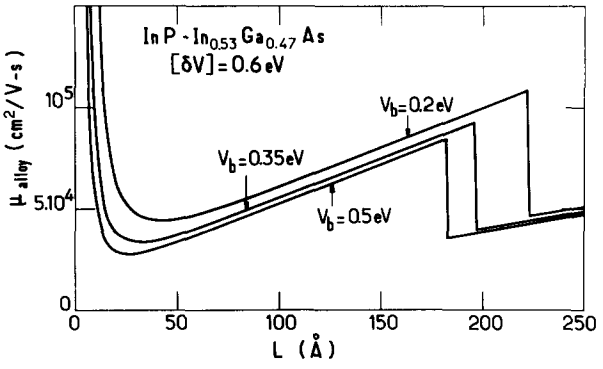

Fig. 3. Mobility limited by alloy scattering versus well thickness in single InP-$In_{0.53}Ga_{0.47}As$ quantum well. Inter-subbands scattering is considered and three values of V_b are used ($V_b = 0.2$ eV, 0.35 eV and 0.5 eV).

(i) The mobility figures are quite insensitive to the precise values of V_b, at least in the E.Q.L. and if $L \gtrsim 50$ Å. To the extent that the band bending can be treated in perturbation, the mobility does not depend on the value of the transferred charge, a feature which contrasts with the results obtained in single H.J. where $\mu_{\text{alloy}} \sim n_e^{-1/3}$.

(ii) the alloy scattering-limited mobility diverges when $L \to 0$. This is associated with the increased leakage of $\psi_1^{(0)}$ wavefunction in InP where alloy scattering does not take place. At large L (still such that the E.Q.L. is justified) μ_{alloy} increases almost linearly with L. This could have anticipated from equation (10) and merely reflects the increased delocalization of $\psi_1^{(0)}$ over the Q.W. and thus its increased insensitivity to spatial fluctuations occurring on a fixed scale (the V.C.A. unit cell). The minimum value for μ_{alloy} which takes place between $L \sim 25$ Å ($V_b = 0.5$ eV) and $L \sim 40$ Å ($V_b = 0.2$ eV) is due to the finite value of V_b: were V_b infinite μ_{alloy} would drop to zero at $L = 0$. Finally when the second Q.W. subband becomes populated the intersubband scattering becomes operative and the mobility drops down to a value which is rather close from the minimum value between 25 Å and 40 Å.

(iii) The exact mobility figure depends on the value of $[\delta V]$ and on "geometrical" factors governing the shape of $\psi_1^{(0)}(z)$. As for $[\delta V]$ we took the value determined by Hayes *et al.* [6] in bulk materials. The importance of "geometrical" factors are more easily discussed if we compare the alloy scattering mobility in a single H.J. and in a M.D.Q.W., all other parameters being fixed (Ω_0, $[\delta V]$. m^* . . .). We see that a typical M.D.Q.W. displays a lower mobility than a typical H.J. Let us take $n_e = 4 \times 10^{11}$ cm^{-2} in both cases and $L = 100$ Å. There is $\mu_{\text{MDQW}} \sim 5 \times 10^4$ cm^2 (Vs)$^{-1}$ (Fig. 3) and from [2] $\mu_{\text{HJ}} \sim 2 \times 10^5$ cm^2 (Vs)$^{-1}$. The larger mobility in single H.J. reflects the larger spreading of the ground state wavefunction. It is due to the smallness of the channel self consistent potential as compared with the potential of the confining barriers in M.D.Q.W.

The alloy scattering in InP-$Ga_{1-x}In_xAs_yP_{1-y}$, $y \neq 0$ can be calculated along the same line as developed for InP-$Ga_{1-x}In_xAs$. However the mobility figures, although smaller than found in InP-$Ga_{1-x}In_xA$, are very imprecise due to the lack of knowledge of V_b and $[\delta V]$ in the quaternary alloys. For a well thickness $L = 150$ Å with $y = 0.5$ and $x = 0.77$ and assuming $V_b = 0.5$ eV the mobility limited by alloy scattering in InP-$Ga_{1-x}In_xAs_yP_{1-y}$ is 1.4×10^4 cm^2 (Vs)$^{-1}$ if $[\delta V]$ is taken from the energy gap difference [7] and 3.8×10^4 cm^2 (Vs)$^{-1}$ if $[\delta V]$ is taken from the electron affinity difference [7].

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