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Alloy scattering-limited mobility in narrow quantum wells

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Alloy scattering-limited mobility is calculated for narrow quantum wells of $GaAs/Ga_{0.7}Al_{0.3}As$, $Ga_{0.47}In_{0.5}As/InP$, and $Al_{0.48}In_{0.5}As/Ga_{0.47}In_{0.53}As$ systems with widths down to 0.5 nm, taking into account the energy-band nonparabolicity and the effects of wave-function penetration into the barrier layer. Values of mobility are found to be significantly different from those given by the formulas derived earlier for wide wells.

Electrons are not fully confined in narrow quantum wells as the wave function extends significantly into the barrier layer for finite barrier potentials. Electrons spend part of the time in the barrier layer in such wells. It has been shown[1] that the partial confinement causes a very large increase in the acoustic-phonon scattering-limited mobility for well widths smaller than 3 nm. However, alloy scattering is more important than acoustic-phonon scattering in quantum wells of mixed compounds.[2] It is independent of temperature and limits the mobility in such wells at low temperatures where phonon scattering is less important. Alloy scattering may be important also in narrow quantum wells of binary compounds, even though it is absent in wide wells of such compounds. When the electrons are partially in the barrier layer, they may be scattered by the alloy potentials in the barrier, the material of which may be a mixed compound. It is, therefore, of interest to study how alloy scattering-limited mobility is affected by the width of the wells for narrow wells. The purpose of this letter is to make such a study for the three quantum-well structures of current interest, namely, $GaAs/Ga_{0.7}Al_{0.7}As$, $Ga_{0.47}In_{0.53}As/InP$, and $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.52}As$.

Alloy scattering being elastic, its effect may be evaluated by using the relaxation-time approximation,[3] which gives the following expression for the mobility μ when only one subband is occupied by the electrons:

$$\mu=-|e|\int [m_e(E)/m_v(E)][1/S(E)](\partial f_0/\partial E)E\,dE \times\left(\int m_v(E)f_0 dE\right)^{-1}, \tag{1}$$

where e is the charge of an electron, f_0 is the equilibrium distribution function for the electrons, $S(E)$ is the total scattering rate for an electron of kinetic energy E, $m_e(E)$ and $m_v(E)$ are, respectively, the energy and the velocity effective mass, given by

$$m_e(E)=\hbar^2k_\parallel^2/2E, \quad m_v(E)=\hbar^2k_\parallel/(\partial E/\partial k), \tag{2}$$

where $k_\parallel$ is the in-plane wave vector corresponding to E.

The two masses of Eq. (2) are given for bulk semiconductors by $m^*(1+\alpha E)$ and $m^*(1+2\alpha E)$, when the Kane dispersion relation,[3] given below, is obeyed

$$\hbar^2k_\parallel^2/2m^*=E(1+\alpha E), \tag{3}$$

where m^* is the band-edge mass and α is the nonparabolicity parameter. The bulk dispersion relation may be taken to be valid for wide wells, but it is modified for narrow wells due to the penetration of the wave function into the barrier layer. The values of $m_e(E)$ and $m_v(E)$ may be obtained for such wells by finding the energy eigenvalues for an in-plane wave vector $\mathbf{k}_\parallel$ as explained in Ref. 1.

Potentials causing the alloy scattering are assumed to be discontinuities of spherical shape in the crystal potential. The magnitude of the discontinuity and radius of the sphere are assumed to be $E_1(z_0)$ and $r_0(z_0)$ when the scattering center is at z_0. The potential may be expressed as a three-dimensional Fourier series in $\mathbf{q}$ as

$$\Delta v=\sum_{\mathbf{q}}(4\pi/3)E_1(z_0)r_0^3(z_0)\exp(i\mathbf{q}_\parallel\cdot\mathbf{r})\exp[iq_z(z-z_0)], \tag{4}$$

where $\mathbf{r}$ is the in-plane position vector, z is the direction perpendicular to the quantum well interfaces, $\mathbf{q}_\parallel$ and q_z are the in-plane and z components of $\mathbf{q}$. The volume of the sample is taken to be unity.

The matrix element for scattering is

$$\langle\Psi^*|\Delta v|\Psi\rangle=\sum_{\mathbf{q}_\parallel,q_z}\int_{-\infty}^{\infty}F'(z)\Delta v(\mathbf{q}_\parallel,q_z)F(z) \times\exp[i(\mathbf{k}_\parallel-\mathbf{k}'_\parallel)\mathbf{r}]\,dr\,dz. \tag{5}$$

where $\mathbf{k}'_\parallel$, $\mathbf{k}_\parallel$ are the in-plane electron wave vectors, Ψ', Ψ are the wave functions, and $F'(z)$, $F(z)$, are the envelope functions corresponding to the $\mathbf{k}'_\parallel$ and $\mathbf{k}_\parallel$ state. It may be noted that only the envelope function components of Ψ have been retained. The cell periodic parts are ignored, as these are assumed to be independent of $k_\parallel$ in the envelope function approximation.

On using Eqs. (4) and (5), the matrix element reduces to

$$\langle\Psi'^*|\Delta v|\Psi\rangle=(4\pi/3)E_1(z_0)r_0^3(z_0)|F(z_0)|^2, \tag{6}$$

since the integral has a nonzero value only for $\mathbf{k}_\parallel-\mathbf{k}'_\parallel+\mathbf{q}_\parallel=0$. The probability of scattering from the $\mathbf{k}_\parallel$ state to $\mathbf{k}'_\parallel$ state is hence given by

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TABLE I. Physical constants.

Material	Lattice constant (Å)	Effective mass ratio	Nonparabolicity parameter $(eV)^{-1}$	Alloy potential (eV)
GaAs	5.6533	0.067	0.885	0
$Ga_{0.7}Al_{0.3}As$	5.6533	0.090	0.631	1.56
InP	5.8688	0.078	0.83	0
$Ga_{0.47}In_{0.53}As$	5.8688	0.042	1.167	0.55
$Al_{0.48}In_{0.52}As$	5.8688	0.08	0.571	0.4,1.3

$$S(\mathbf{k}_{\parallel},\mathbf{k}'_{\parallel}) = (2\pi/\hbar)\int [(4\pi/3)E_1(z_0)r_0^3(z_0)]^2 \times |F(z_0)|^4 x(1-x)(N/2)\delta(E'-E)dz_0 = \int c_{\mathrm{all}}(z_0)|F(z_0)|^4\delta(E'-E)dz_0, \quad (7)$$

where

$$c_{\mathrm{all}}(z_0) = (2\pi/\hbar)[(4\pi/3)E_1(z_0)r_0^3(z_0)]^2 x[1-x]N/2, \quad (8)$$

and E' and E are the kinetic energies corresponding respectively to $\mathbf{k}'_{\parallel}$ and $\mathbf{k}_{\parallel}$. The concentration of scattering centers is taken to be independent of z_0 and given by $x(1-x)N/2$, where N is the number of atoms per unit volume of the crystal, and x is the value of the fraction in a material with the symbol $A_xB_{1-x}C$.

On using Eq. (7), the total scattering rate $S(E)$ is found to be

$$S(E) = (1/2\pi\hbar^2)m_v(E)\int_{-\infty}^{\infty} c_{\mathrm{all}}(z_0)|F(z_0)|^4 dz_0. \quad (9)$$

Mobilities have been calculated for the GaAs/$Ga_{0.7}Al_{0.3}As$, $Ga_{0.47}In_{0.53}As$/InP, and $Ga_{0.47}In_{0.53}As$/$Al_{0.48}In_{0.52}As$ wells of widths between 0.5 and 10 nm, by using the values of the physical constants given in Table I. Potential barriers for the GaAs/GaAlAs, GaInAs/InP and GaInAs/AlInAs were taken, respectively, as 0.275, 0.24, and 0.5 eV. Values of mobility are presented in Fig. 1.

Alloy scattering is usually neglected for the GaAs/GaAlAs system, since the well material is a binary compound and has no alloy disorder. It is, however, found that though the contribution of alloy scattering may be considered negligible for wide wells, it starts being significant for quantum wells narrower than 10 nm. Electron mobility of 165 m^2/V s has been reported[5] for a single-heterojunction well of GaAs/GaAlAs, the effective width of which works out to be about 20 nm. Present calculations, using an alloy potential[6] of 1.56 eV for $Ga_{0.7}Al_{0.3}As$, indicate that such high mobilities will not be obtained for double-heterojunction wells if the width is made small. Alloy scattering which is independent of temperature, has a considerable contribution from about 10 nm and limits the mobility to much lower values.

Alloy scattering limits also the low temperature electron mobility in the GaInAs/InP system. It produces a mobility of about 4 m^2/V s for a 10-nm-thick well. The mobility decreases approximately as the inverse of the well width down to about 4 nm as expected from the theory,

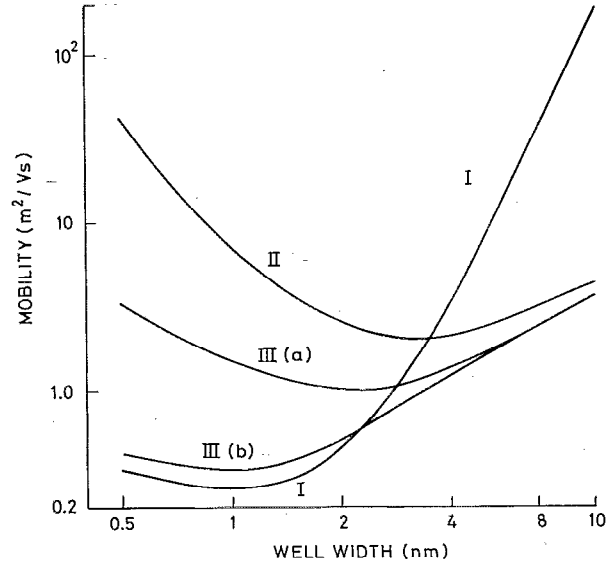

FIG. 1. Well-width dependence of alloy scattering-limited mobility in GaAs/GaAlAs, GaInAs/InP, and GaInAs/AlInAs quantum wells. I—GaAs/$Ga_{0.7}Al_{0.3}As$; II—$Ga_{0.47}In_{0.53}As$/InP; III(a)—$Ga_{0.47}In_{0.53}As$/$Al_{0.48}In_{0.52}As$, E_1(AlInAs) = 0.4 eV; III(b)—$Ga_{0.47}In_{0.53}As$/$Al_{0.48}In_{0.52}As$, E_1(AlInAs) = 1.3 eV.

neglecting the effects of finite barrier height. The present calculations, however, indicate a new feature that the mobility increases with decrease in the well width and has a very large value for wells narrower than 1 nm. The increase is due to the extension of the wave function into the InP layer, in which there is no alloy scattering. It may also be noted that our calculated value of alloy scattering-limited mobility for the well of 10-nm width is lower by a factor of about 4 in comparison to the value calculated earlier.[7] This difference is partly due to using the latest value,[2] 0.55 eV, for the alloy potential instead of 0.42 eV, estimated earlier.[8] It is also partly due to a difference of a factor of 3/4 in our formula with that derived earlier by using an alloy potential of a cylindrical geometry. The inclusion of band nonparabolicity in our analysis has also lowered the value of mobility.

Alloy scattering-limited mobility in the GaInAs/AlInAs system has been calculated by using two values of alloy potentials[9] for AlInAs, 0.4 and 1.3 eV, since no established value is available and these two values appear to be the extreme limits. Lowering of the values of mobility for this system in comparison to those for $Ga_{0.47}In_{0.53}As$/InP wells may be understood by considering that the energy eigenvalues are higher in this system due to higher barrier potential and the effect of nonparabolicity is larger. It is also seen that for the potential of 0.4 eV, the mobility decreases approximately as $1/L$ (L is the well width) down to about 3 nm, but for lower widths, it increases and the value for 0.5 nm is nearly the same as that for a 10-nm well. On the other hand, for an alloy potential of 1.3 eV for AlInAs, the mobility decreases faster than $1/L$ down to the lowest width. These distinctive features are as expected. The difference in the two cases arises from the effects of

wave-function penetration into the barrier which increases with decrease in the well width. This characteristic may be used fruitfully to estimate the alloy potential in $Al_{0.48}In_{0.52}As$.

In summary, the extension of the wave function into the barrier layer for narrow quantum wells with finite barrier height, changes significantly the alloy scattering-limited mobility. The mobility is reduced by orders of magnitude and becomes comparable to that limited by other scattering mechanisms in GaAs/GaAlAs wells. It is reduced also in GaInAs/AlInAs wells for the assumed value of 1.3 eV for the alloy potential in AlInAs. On the other hand, it is significantly increased in very narrow wells of the GaInAs/InP system and also in the GaInAs/AlInAs system for the value of 0.4 eV for the alloy potential in AlInAs.

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