Alloy scattering in quantum-well structures of semiconductor ternaries

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An expression for the relaxation time due to alloy scattering in the quantum-well structure of a semiconductor ternary is derived. The resulting mobility of the two-dimensional electron gas in the well is found to be independent of temperature. Considering $Ga_{0.47}In_{0.53}As$, it is shown that the alloy-scattering mobility in a thick quantum well may exceed that in a highly degenerate bulk material at not too low temperatures.

Recent advances in crystal growth have produced very thin layers of semiconductors forming quantum wells between parallel potential barriers separated by some tens of angstroms. Such structures possess extremely high electron mobility at low temperatures since the electrons may be spatially separated from their parent donor atoms.¹ While a GaAs quantum well is the subject of many investigations, quantum wells of semiconductor ternaries like $Ga_{1-\alpha}In_{\alpha}As$ are also receiving attention.² In ternary structures, mobility is affected by alloy scattering, which is an intrinsic process arising from the random distribution of the alloy atoms in the available lattice points.³ We consider this scattering mechanism here for the two-dimensional electron gas in the quantum-well structure of a ternary alloy and derive an expression for the relaxation time. The alloy-scattering mobility, found here to be temperature independent, may be the ultimate source limiting the mobility in quantum wells.

We consider a quantum well of an alloy denoted by the symbol $A_{1-\alpha}B_{\alpha}C$. The thickness of the well is L, i.e., the confining parallel potential barriers are at a length L apart. Assuming that the electrons are in the lowest subband, the normalized wave function is given by⁴

$$\psi(\vec{\mathbf{r}},z) = \left(\frac{2}{V}\right)^{1/2} u_{\vec{\mathbf{k}}}(\vec{\mathbf{r}},z) \exp(i\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}) \sin\left(\frac{\pi z}{L}\right) , \quad (1)$$

where the z direction is normal to the plane of the potential barriers, \vec{r} is a two-dimensional position vector in the (x,y) plane, V is the volume of the well, \vec{k} is the component of the wave vector \vec{K} in the (x,y) plane, and $u_{\vec{K}}$ is the Bloch function.

The electron energy in the state \vec{k} is

$$E_k = E_0 + \frac{\hbar^2 k^2}{2m^*} , \qquad (2)$$

where

$$E_0 = \frac{\hbar^2 \pi^2}{2m^* L^2} , \qquad (3)$$

 \hbar is Planck's constant divided by 2π , and m^* is the effective mass.

We consider the virtual-crystal potential to be perfectly periodic as it is composed of the composition-weighted potentials due to the A and B atoms. The difference between the actual crystal potential and the virtual-crystal potential is the scattering potential, which is assumed³ to have a magnitude ΔE and a range r_0 . Using the Born approximation and taking the overlap factor to be unity, the matrix element of transition from state \vec{k} to $\vec{k'}$ is

$$|m(\vec{k},\vec{k}')| = \frac{2}{V} \Delta E \int_0^{r_0} \int_0^{2\pi} \int_{z_j - r_0}^{z_j + r_0} \exp[i(\vec{k} - \vec{k}') \cdot \vec{r}] \sin^2\left(\frac{\pi z}{L}\right) r \, dr \, d\theta \, dz \quad , \tag{4}$$

where z_j is the z coordinate of the scattering site. The range of the scattering potential is somewhat arbitrary, but a good choice for r_0 is the nearest-neighbor distance,³ which for a zinc-blende structure of lattice parameter "a" is $\sqrt{3}a/4$. As a is about 5 or 6 Å, $r_0 \approx 2.5 \times 10^{-10}$ m. Also,

$$|\vec{\mathbf{k}} - \vec{\mathbf{k}}'|_{\text{max}} \simeq 4(m^* k_B T/\hbar^2)^{1/2} \simeq 2.7 \times 10^7 \times T^{1/2} \text{ (m)}^{-1}$$

for $m^* = 0.04m_0$, where m_0 is the electron rest mass. Hence $|\vec{k} - \vec{k}'|_{\max} r_0 \approx 6.8 \times 10^{-3} \times T^{1/2}$ so that $(\vec{k} - \vec{k}') \cdot \vec{r}$ in Eq. (4) may be taken to be much smaller than unity at ordinary temperatures. Also, since L is at least some tens of angstroms, we may assume $r_0 \ll L$. With these approximations, Eq. (4) reduces to

$$|m(\vec{\mathbf{k}},\vec{\mathbf{k}}')| \simeq \frac{2\pi r_0^3 \Delta E}{V} \quad . \tag{5}$$

The square of the transition matrix element $|M(\vec{k}, \vec{k}')|^2$

determining the scattering rate is obtained by summing $|m(\vec{k}, \vec{k}')|^2$ over all the scattering sites. The number of such sites in a volume element Sdz is given by $\alpha(1-\alpha) \times SNP_0dz/2$, where S is the surface area in the (x,y) plane, N is the number of lattice points per unit volume available to the A or B atoms, and P_0 is a parameter describing the amount of ordering in the alloy.⁵ In general, P_0 lies between 0 and 1; for a completely random alloy, $P_0=1$. Thus

$$|M(\vec{k}, \vec{k}')|^{2} = \left(\frac{2\pi r_{0}^{3}\Delta E}{V}\right)^{2} \alpha(1-\alpha) \frac{SNP_{0}}{2} \int_{0}^{L} dz$$
$$= \frac{2\pi^{2} r_{0}^{6} |\Delta E|^{2} \alpha(1-\alpha) NP_{0}}{V}$$
$$= \frac{27\pi^{2} \alpha(1-\alpha) |\Delta E|^{2} P_{0}}{128 VN} , \qquad (6)$$

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since $N = 4/a^3$ and $r_0 = \sqrt{3}a/4$. If τ is the relaxation time, we have

$$\frac{1}{\tau} = \frac{S}{(2\pi)^2} \int \frac{2\pi}{\hbar} |M(\vec{k}, \vec{k}')|^2 \delta(E_{\vec{k}} - E_{\vec{k}'}) d\vec{k}' , \quad (7)$$

where $d\vec{k}' = k' dk' d\beta$, β is the angle between \vec{k} and \vec{k}' , and $\delta(x)$ is the Dirac δ function signifying conservation of electron energy. Performing the β integration, converting from k' to $E_{k'}$, and using the property of the δ function, we have for a completely random alloy

$$\frac{1}{\tau} = \frac{27\pi^2 \alpha (1-\alpha) m^* |\Delta E|^2}{128 N L \hbar^3} .$$
(8)

Note that τ is proportional to the thickness of the well and is inversely proportional to the effective mass, but is independent of electron energy or temperature. The alloyscattering mobility in a quantum well is therefore temperature independent and is given by

$$\mu = \frac{e\tau}{m^*} = \frac{128eNL\hbar^3}{27\pi^2\alpha(1-\alpha)m^{*2}|\Delta E|^2} , \qquad (9)$$

where e is the electron charge. For a well of Ga_{0.47}In_{0.53}As of thickness 100 Å, using⁶ $N = 1.98 \times 10^{28} \text{ m}^{-3}$, $m^* = 0.041m_0$, and $\Delta E = 0.42 \text{ eV}$, we obtain $\mu = 1.1 \times 10^5 \text{ cm}^2 \text{ V}^{-1} \text{ sec}^{-1}$. This is the limiting mobility in the ideal case at very low temperatures where phonon scattering is negligible and impurity scattering is also reduced by spatial separation of the donors. Mobilities around $1.8 \times 10^4 \text{ cm}^2 \text{ V}^{-1} \text{ sec}^{-1}$ have been reported for Ga_{0.47}In_{0.53}As quantum wells at 77 K.²

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In the bulk material, alloy-scattering relaxation time is inversely proportional to the square root of electron energy and to the three-halves power of the effective mass.³ If μ_0 be the alloy-scattering mobility in the bulk material, then for a nondegenerate (n. deg.) electron distribution we have

$$\left(\frac{\mu}{\mu_0}\right)_{\text{n. deg.}} = 0.36 \times T^{1/2} \left(\frac{L}{100}\right) \left(\frac{m^*}{m_0}\right)^{1/2} , \qquad (10)$$

where L is in angstroms. For Ga_{0.47}In_{0.53}As with L = 100 Å, we obtain $(\mu/\mu_0)_{n. deg.} = 0.07 \times T^{1/2}$, so that the alloyscattering mobility in the quantum well is less than that in the bulk at temperatures below 204 K.

On the other hand, for a completely degenerate electron distribution we have

$$\left(\frac{\mu}{\mu_0}\right)_{\text{deg.}} = 0.27 \times T^{1/2} \left(\frac{L}{100}\right) \left(\frac{m^*}{m_0}\right)^{1/2} \left(\frac{E_F}{k_B T}\right)^{1/2} , \qquad (11)$$

where E_F is the Fermi energy in the bulk material, k_B is the Boltzmann constant, and L is in angstroms. For Ga_{0.47}In_{0.53}As, with L = 100 Å and $E_F = 4k_BT$, we find $(\mu/\mu_0)_{deg} = 0.11 \times T^{1/2}$, so that the quantum-well mobility is higher than the bulk value for temperatures above 83 K. Doubling the thickness of the well will reduce this temperature 4 times. Thus, improvements over mobilities in degenerate bulk samples are possible for thicker wells at not too low temperatures.

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