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Interface roughness scattering in a superlattice

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Abstract. We examine the role of interface roughness (IFR) scattering in electron transport in a GaAs/GaAlAs superlattice, using a simple model. The IFR is assumed to be small, slowly varying and to be characterised by a height and a lateral size. In contrast with previous studies of IFR scattering we take the barrier height to be finite. We find that the use of an infinite barrier approximation leads to large errors. We use Fermi's golden rule to calculate scattering rates and the Boltzmann transport equation to calculate IFR scattering-limited mobility in the growth direction at 300 K for a low density non-degenerate electron gas. We find that the mobility limited by IFR scattering is up to an order of magnitude less than the predicted LO phonon scattering-limited mobility.

1. Introduction

It has been shown experimentally that in GaAs/GaAlAs superlattices having thin enough barriers electron transport in the growth direction proceeds by extended Bloch states [1–3]. A few authors have calculated the electron mobility in the growth direction at room temperature using Boltzmann transport theory and assuming LO phonons as the dominant scattering mechanism [4–6]. However the theoretically calculated mobilities are about an order of magnitude larger than the experimental values. This suggests the prevalence of other scattering mechanisms. Moreover the electron–LO phonon interaction is weakened in a superlattice due to the effect of the superlattice structure on the optical phonon modes [6].

In this paper we examine the role of interface roughness (IFR) scattering on the electron transport. Although extensive studies have been made of the IFR scattering for Si metal-oxide–semiconductor inversion layers [7], very little work has been done for GaAs/GaAlAs superlattices. However, in a superlattice, IFR may be expected to be particularly important because only a small change of barrier width can cause a large fluctuation of the mini-band width.

The exact nature of the IFR is unknown. Consequently the interface scattering is studied within a simple model [8]. The IFR is assumed to be small, slowly varying and to be characterised by a height Ω and a lateral size Λ. We use Fermi's golden rule to calculate scattering rates and the Boltzmann transport equation to calculate IFR scattering-limited mobilities in the growth direction at 300 K. These results are compared with previous calculations that take LO phonons as the dominant scattering mechanism. Attention is focused on low doping levels so that screening and interband scattering can be neglected.

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2. Electrons

Effective mass theory is used to calculate the mini-band structure and envelope function of the electron states. For simplicity the small difference in effective mass between the GaAs and GaAlAs layers is ignored. The superlattice potential is of the Kronig–Penney type with the same periodicity as the superlattice (see figure 1). In the manner of [4–6] the mini-band dispersion is represented by the phenomenological form

$$\epsilon_k = \frac{\hbar^2 k_\parallel^2}{2m^*} + \Delta(1 - \cos k_z l) \tag{1}$$

where 2Δ is the mini-band width obtained from the Kronig–Penney model. The barrier height is taken to be 250 meV which corresponds to $x = 0.3$ in the $Al_xGa_{1-x}As$ layer [9].

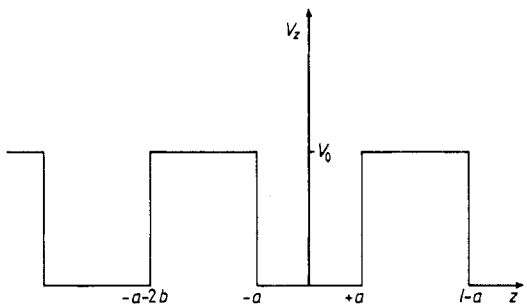

Figure 1. The Kronig–Penney potential.

The envelope function is written in the tight-binding formalism as

$$\Psi_k = \left(\frac{l}{V}\right)^{1/2} \exp(i\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel) \sum_{n=-N/2}^{n=+N/2} \phi(z - nl) \exp(ik_z nl) \tag{2}$$

where $\boldsymbol{k}_\parallel = k_x\hat{\boldsymbol{i}} + k_y\hat{\boldsymbol{j}}$, $\boldsymbol{x}_\parallel = x\hat{\boldsymbol{i}} + y\hat{\boldsymbol{j}}$ and $\phi(z)$ is the normalised eigenfunction of the Hamiltonian for a single potential well of width $2a$ and barrier height 250 meV centred at z=0. The normalisation constant in (2) is determined by making use of

$$\phi(z - nl)\phi(z - ml) = \delta_{n,m}\phi^2(z - nl). \tag{3}$$

3. Interface roughness scattering

Experimental evidence shows that the form of the IFR of AlGaAs grown on GaAs surface can be different from that of GaAs on AlGaAs [10–12]. Thus we treat scattering from the two types of interfaces separately, and use the subscript $i = 1$ for GaAs grown on AlGaAs and subscript $i = 2$ for AlGaAs on GaAs. If the deviation of the interface

at $z = nl + a$ (GaAs on AlGaAs) from a flat plane is given by $\Omega_1^n(x,y)$ then it's scattering potential for the IFR is

$$H_{1_{SR}}^n = \begin{cases} V_0 & nl + a + \Omega_1^n(x,y) < z < nl + a \qquad \Omega_1^n(x,y) < 0 \\ -V_0 & nl + a < z < nl + a + \Omega_1^n(x,y) \qquad \Omega_1^n(x,y) > 0 \\ 0 & \text{otherwise} \end{cases} \tag{4}$$

where V_0 is the barrier potential height and SR means surface roughness. The deviation of the interface at $z = nl - a$ (AlGaAs on GaAs) from a flat plane is given by $\Omega_2^n(x,y)$, and it's scattering potential $H_{2_{SR}}^n$ is written in a similar manner to (4). The total scattering potential, including the contribution from all the interfaces is then given by

$$H_{SR} = \sum_{i=1}^{2} \sum_{n} H_{i_{SR}}^n. \tag{5}$$

The IFR is taken to be small and slowly varying and we assume a Gaussian form of the correlation of the IFR. Thus the autocorrelation function is written as

$$\langle \Omega_i^n(x,y) \Omega_j^m(x',y') \rangle = \delta_{n,m}\, \delta_{i,j}\, \Omega_i^2 \exp[-\Lambda_i^{-2}(\boldsymbol{x}_{\|} - \boldsymbol{x}'_{\|})^2]. \tag{6}$$

Using (6) the square of the scattering matrix element is found to be

$$|\langle \boldsymbol{k} \mid H_{SR} \mid \boldsymbol{k}' \rangle|^2 = \pi V_0^2 \frac{l}{V} \phi^4(a) \sum_{i=1}^{2} \Omega_i^2 \Lambda_i^2 \exp\left(-\frac{\Lambda_i^2}{4}(\boldsymbol{k}'_{\|} - \boldsymbol{k}_{\|})^2\right). \tag{7}$$

In deriving (7) we ignore inter-well scattering, i. e. make use of (3). Using the Fermi golden rule the scattering rate is then given as

$$T(\boldsymbol{k}, \boldsymbol{k}') = \frac{2\pi^2 l}{\hbar V} V_0^2 \phi^4(a) \sum_{i=1}^{2} \Omega_i^2 \Lambda_i^2 \exp\left(-\frac{\Lambda_i^2}{4}(\boldsymbol{k}'_{\|} - \boldsymbol{k}_{\|})^2\right) \delta(\epsilon - \epsilon'). \tag{8}$$

The reciprocal of the electron lifetime

$$\begin{aligned} \tau^{-1}(\boldsymbol{k}) &= \frac{V}{8\pi^3} \int T(\boldsymbol{k}, \boldsymbol{k}')\, \mathrm{d}^3\boldsymbol{k}' \\ &= \frac{l}{4\pi\hbar} V_0^2 \phi^4(a) \sum_{i=1}^{2} \Omega_i^2 \Lambda_i^2 \int_{-\pi/l}^{\pi/l} \mathrm{d}k'_z \int \exp\left(-\frac{\Lambda_i^2}{4}(\boldsymbol{k}'_{\|} - \boldsymbol{k}_{\|})^2\right) \delta(\epsilon - \epsilon')\, \mathrm{d}^2\boldsymbol{k}'_{\|}. \end{aligned} \tag{9}$$

In contrast with previous studies of IFR scattering we have not taken the barrier height V_0 to be infinite. While the approximation of infinite barrier height is adequate for Si MOSFETS and GaAs/AlAs heterostructures, we find it leads to large errors in a $GaAs/Ga_{0.7}Al_{0.3}As$ system where the barrier height is only 250 meV. The IFR scattering is proprtional to $V_0^2\phi^4(a)$, and using

$$\phi(a) = \left(\frac{\hbar^2}{2m^*(V_0 - E_0)}\right)^{1/2} \frac{\mathrm{d}\phi}{\mathrm{d}z}\bigg|_{z=a} \tag{10}$$

we obtain

$$V_0^2\phi^4(a) = \frac{\hbar^4 V_0^2}{4m^{*2}(V_0 - E_0)^2} A^4 k_0^4 \sin^4 k_0 a. \tag{11}$$

For an infinte barrier height $A = a^{-1/2}$ and $k_0 a = \pi/2$. We can see why the infinite barrier approximation leads to large errors by taking an example: a finite well of width 30 Å and barrier height 250 meV. In this case $E_0 = 137$ meV and the gradient of $\phi(z)$ at $z = a$ is one quarter of that predicted for an infinte potential well. Since in (11) we take the gradient to the fourth power this difference is considerably magnified. Consequently the use of the infinite barrier height approximation would overestimate the scattering by two orders of magnitude. As the well width is increased this difference is reduced. For a well of width 50 Å the infinite barrier height would overestimate the scattering by one order of magnitude.

A recent study of IFR scattering in quantum wells used as the scattering potential, the fluctuations in the lowest energy level of an infinite potential well due to variations in the well width [10]. Proceeding similarly we may write

$$H_{\mathrm{SR}} = \frac{\partial E_0}{\partial L_{\mathrm{W}}}[\Omega_1(x,y) - \Omega_2(x,y)]. \tag{12}$$

E_0 is the lowest energy level for an infinite quantum well, L_{W} is the well width and $\Omega_1(x,y) - \Omega_2(x,y)$ is the change in the well width due to the IFR. Making use of the autocorrelation function, the average scattering rate for quasi-2D free electrons in an xy plane of area A is

$$T(\boldsymbol{k}_{\|}, \boldsymbol{k}'_{\|}) = \frac{2\pi^6\hbar^3}{A(m^*)^2 L_{\mathrm{W}}^6} \sum_{i=1}^{2} \Omega_i^2 \Lambda_i^2 \exp\left(-\frac{\Lambda_i^2}{4}(\boldsymbol{k}'_{\|} - \boldsymbol{k}_{\|})^2\right) \delta(\epsilon - \epsilon'). \tag{13}$$

We can see that in this case the scattering rate is proprtional to L_{W}^{-6}, this means that IFR scattering is much more important for narrow wells and the IFR scattering limited mobility in quantum wells is proportional to L_{W}^6 [10]. The reciprocal of the electron lifetime can then be calculated as

$$\begin{aligned}\tau^{-1}(\boldsymbol{k}) &= \frac{A}{4\pi^2} \int T(\boldsymbol{k}_{\|}, \boldsymbol{k}'_{\|})\, \mathrm{d}^2\boldsymbol{k}'_{\|} \\ &= \frac{\pi^4\hbar^3}{2(m^*)^2 L_{\mathrm{W}}^6} \sum_{i=1}^{2} \Omega_i^2 \Lambda_i^2 \int \exp\left(-\frac{\Lambda_i^2}{4}(\boldsymbol{k}'_{\|} - \boldsymbol{k}_{\|})^2\right) \delta(\epsilon - \epsilon')\, \mathrm{d}^2\boldsymbol{k}'_{\|}\,. \end{aligned} \tag{14}$$

It is interesting to compare the results of the two models. Thus if we take the limit $V_0 \to \infty$ (the mini-band width $2\Delta \to 0$)

$$\lim_{V_0 \to \infty} V_0^2 \phi^4(a) = \frac{\pi^4\hbar^4}{(m^*)^2(2a)^6} \tag{15}$$

then (9) becomes

$$\tau^{-1}(\boldsymbol{k}) = \frac{\pi^4\hbar^3}{2(m^*)^2(2a)^6} \sum_{i=1}^{2} \Omega_i^2 \Lambda_i^2 \int \exp\left(-\frac{\Lambda_i^2}{4}(\boldsymbol{k}'_{\|} - \boldsymbol{k}_{\|})^2\right) \delta(\epsilon - \epsilon')\, \mathrm{d}^2\boldsymbol{k}'_{\|}\,. \tag{16}$$

This is identical to (14), reproducing the L_{W}^{-6} dependence.

4. Calculation of mobility

Since the electrons are assumed to have extended Bloch states, Boltzmann transport theory is used. If a small electric field is applied to the superlattice perpendicular to the layers, the electron distribution function can be written as

$$f = f_0 + g \tag{17}$$

where f_0 is the Fermi-Dirac distribution and g is the first order perturbation. The IFR scattering is k_z randomising, i.e.

$$T(\boldsymbol{k}_{\|}, k_z : \boldsymbol{k}'_{\|}, k'_z) = T(\boldsymbol{k}_{\|}, k_z : \boldsymbol{k}'_{\|}, -k'_z) \tag{18}$$

so the relaxation time approximation can be used when the electric field is applied in the z-direction. Thus, using the linearised Boltzmann equation and assuming non-degenerate statistics so that $f_0 \ll 1$ we have

$$g(\boldsymbol{k}) = \tau_r(\boldsymbol{k}) \frac{e}{\hbar} E_z \frac{\partial f_0}{\partial k_z} \tag{19}$$

where

$$\tau_r(\boldsymbol{k}) = \left(\frac{V}{8\pi^3} \int T(\boldsymbol{k}, \boldsymbol{k}') \, \mathrm{d}^3\boldsymbol{k} \right)^{-1}. \tag{20}$$

Then the electron mobility in the direction perpendicular to the layers is given by

$$\mu_z = \frac{j_z}{neE_z} \tag{21}$$

where

$$j_z = -\frac{e}{4\pi^3} \int g(\boldsymbol{k}) v_z(\boldsymbol{k}) \, \mathrm{d}^3\boldsymbol{k} \,. \tag{22}$$

Before the mobility can be evaluated the values of the IFR parameters need to be known. There is good agreement on the value of the height Ω, and this is taken to be one monolayer [10–14]. For the lateral size Λ we use the results of [12]. From RHEED surface diffusion measurements the authors deduce that GaAs grown on AlGaAs surfaces have IFR with lateral width $\Lambda_1 = 35$ Å, AlGaAs on GaAs surfaces have lateral width $\Lambda_2 = 200$ Å. Similar results are obtained from studies of photoluminescence data and measurements of electron mobility in GaAs/AlAs quantum wells [10, 11]. As we show in figure 2, we find that the IFR scattering-limited mobility is less than the LO-phonon limited mobility , and the IFR of the AlGaAs on GaAs surface is mainly responsible for the scattering.

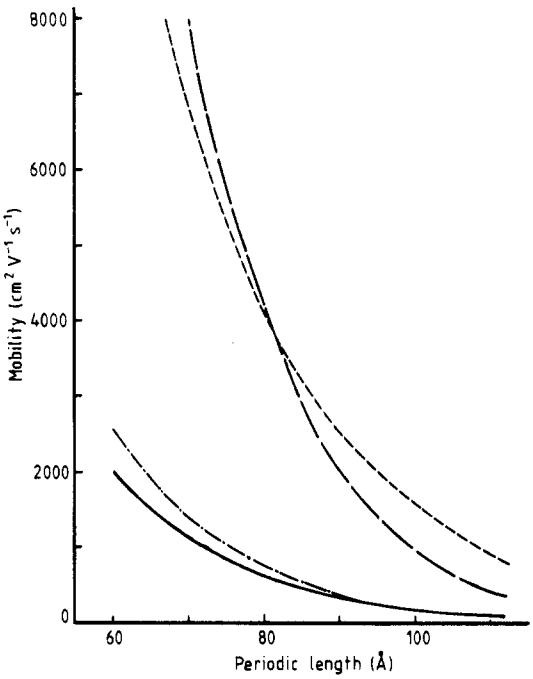

Figure 2. Mobility as a function of superlattice periodic length. ——, total IFR scattering; – – –, IFR scattering from $\Lambda = 35$ Å type interfaces; — · —, IFR scattering from $\Lambda = 200$ Å type interfaces; — — —, LO phonon scattering.

5. Conclusion

In this paper we have shown the importance of IFR scattering at room temperature. We find that the mobility limited by IFR scattering is up to an order of magnitude less than LO phonon scattering-limited mobility (the LO phonon modes are calculated using the dielectric continuum model [6]). Electron mobilities have been measured for some $GaAs/Ga_{0.7}Al_{0.3}As$ superlattices [3]. For a 40 Å/20 Å (well width/barrier width) superlattice the mobility was measured as about 1000 cm^2 V^{-1} s^{-1}. While the IFR scattering-limited mobility gives a much better agreement with experiment than the LO phonon-limited mobility we find it is a factor of five larger than the experimentally measured mobility. There may be a number of reasons for this. The barrier layers of the superlattice are quite narrow and the tight-binding approximation we have used to calculate the envelope functions is likely to be inadequate. Using the correct envelope functions is likely to increase the scattering rate. The scattering rate is also very sensitive to the IFR parameters and a small change in these could also increase it considerably.

References

[1] Devaud B, Shah J, Damen T C, Lambert B and Regemy A 1987 *Phys. Rev. Lett.* **58** 2582
[2] Sibille A, Palmier J and Minot C 1989 *Appl. Phys. Lett.* **54** 165
[3] Sibille A, Palmier J, Minot C, Harmand J and Dubon-chevallier C 1987 *Superlatt. Microstruct.* **3** 553

[4] Palmier J and Chomette A 1982 *J. Physique* **43** 381
[5] Warren G and Butcher P N 1986 *Semicond. Sci. Technol.* **1** 133
[6] Dharssi I and Butcher P N 1990 *J. Phys.: Condens. Matter* **2** 119
[7] Ando T, Fowler A and Stern F 1982 *Rev. Mod. Phys.* **54** 502–6 and references therein
[8] Prange R and Nee T 1968 *Phys. Rev.* **168** 779
[9] Okumara H, Misawa S, Yoshida S and Gonda S 1985 *Appl. Phys. Lett.* **46** 4377
[10] Sakaki H, Noda T, Hirakawa K, Tanaka M and Matsusue T 1987 *Appl. Phys. Lett.* **51** 1934
[11] Tanaka M and Sakaki H 1987 *J. Cryst. Growth* **81** 153
[12] Joyce B A, Dobson P J, Neave J H and Zhang J 1986 *Surf. Sci.* **174** 1; 1986 *Surf. Sci.* **178** 110
[13] Devaud B, Emery J Y, Chomette A, Lambert B and Baudet M 1984 *Appl. Phys. Lett.* **45** 1078
[14] Weisbuch C, Dingle R, Gossard A and Weigmann W 1980 *J. Vac. Sci. Technol.* **17** 1128