CHAPTER 6

CALCULATIONS OF ONE-DIMENSIONAL HOT ELECTRON ac MOBILITY IN GaAs QUANTUM WIRES
6.1. INTRODUCTION:

Advances in the crystal growth techniques like fine line lithography, molecular beam epitaxy (MBE) and metalorganic chemical vapour deposition (MOCVD) have added astonishing possibilities to the fabrication of new artificial materials. In such artificial materials the layer dimensions are comparable to the de Broglie wavelength and hence a subband structure is formed allowing two-dimensional transport of carrier parallel to the interfacial planes. Recently, an alternative structure has been proposed where the electrons are free to move one dimensionally (1D) along the longitudinal direction [6.1]. Such a structure is referred to as quantum wire [QWR]. Much effort has been devoted in recent years to study the properties of QWRs [6.2-6.20]. The quantization of the electron motion in QWRs brings about different features in the electron kinetics compared with the usual three dimensional (3D) electron systems with the same material parameters [6.21]. Electronic transport in one-dimensional (1D) systems is different from that in the two-dimensional (2D) structures and the bulk material because the density - of - states and the scattering rates are different [6.21, 6.22]. Investigations on electronic transport in QWRs are extremely important for an understanding of the basic carrier kinetics and also for the realisation of fast miniature devices [6.23].
In this article, calculations of the ac mobility of 1D degenerate hot electrons in GaAs QWRs are reported when a small-signal sinusoidal electric field superimposed on a dc bias field is applied along the axis of the wire. The results are obtained by solving the energy and momentum balance equations for the carriers including the relevant scattering mechanisms for lattice temperatures of 77 and 300K. The dependencies of ac mobility and the cutoff frequency on various system parameters are studied. The role of the bias field on the cut-off frequency is also investigated.

6.2. LITERATURE SCAN:

Electron-phonon interaction plays a vital role in the physics of electronic transport in semiconductors[6.24]. Such interactions are also important in hot-electron physics, which predicts the behaviour of carriers under high electric fields and hence the characteristics of ultrathin, high field devices. Fabrication of a low-dimensional structure (LDS), confining electrons in a ultra small semiconducting wires has been proposed by Sakaki [6.1, 6.25]. Realisation of such structures and study of their properties have been reported thereafter by different Researchers from time to time [6.26 - 6.35].

The electronic mobility in a QWR in the extreme quantum limit(EQL) was investigated by Sakaki [6.1, 6.25]. He
incorporated in his investigation the ionized impurities located a fixed distance outside the structure. The electronic mobility due to impurity scattering was found to enhance significantly with the distance between the impurities and the wire. It was also reported theoretically that the elastic scattering processes were very effectively reduced in these structures due to only one-dimensional motion of the carriers and thereby enhancing the electronic mobility beyond $10^2 \text{m}^2/(\text{Vs})$ [6.25, 6.36].

Similar studies on QWR in parallel with Sakaki have been done by some other workers too. Arora [6.37] studied the acoustic phonon scattering via deformation potential coupling and the point defect scattering in one-dimensional systems for the rectangular semiconducting wires. He obtained the expressions for the inverse momentum relaxation time for these scatterings. Later on Arora [6.38] reported a quantum theory for electrical conductivity in a thin semiconducting wire of rectangular cross section.

The works of Sakaki [6.1, 6.25] were followed by Petroff et al. [6.39]. They realised GaAs/ $Ga_{1-x}Al_x As$ QWRs with submicron dimensions using MBE and reported several experimental luminescence properties of such structure.

Lee and Spector [6.40] extended Sakaki's model to take into account the scattering in a real quantum-wire structure. They incorporated the effects of background ionized impurities, remote
ionized impurities having somewhat different distribution. In a separate calculation they took an uniform distribution of ionized impurities. They derived expressions for the momentum relaxation time and calculated mobility in these cases for a long cylindrical wire in the size quantum limit (SQL). The relaxation time was found to exhibit a diverse logarithmic variation with the decrease of the radius of the wire. The electron mobility was reported to be reduced with the decrease of radius of the wire. Thus they concluded that for nonuniform ionized impurities, the background impurities could effectively limit the mobility in ultrathin semiconducting quantum-wires. But for uniform distribution of remote impurities both the momentum relaxation time and the mobility were reported to be independent of the transverse dimension of the wire in the SQL.

Later, Lee and Vassell [6.41] generalised Sakaki's treatment to take into account the scattering of carriers in a real QWR semiconductor by both remote and background impurities and also by phonons at finite temperatures. They derived the approximate analytic expressions of momentum relaxation rate for acoustic phonon, polar optic phonon, and background and remote impurity scatterings in a quasi 1D system (Q1D) in the SQL. The expression for momentum relaxation rate by the background ionized impurities was deduced for a 1D system incorporating dielectric function obtained using Thomas-Fermi approximation (TFA). The
low-field drift mobility was calculated numerically in the SQL. They reported that the electron mobility is enhanced in a Q1D system over the mobility in 3D system when the phonon scattering mechanism was the dominant one and when the transverse dimensions of the wire were large enough. However it was pointed out that their model was incorrect at low temperature because of non degeneracy of the carrier distribution and of the TFA.

The dielectric response function for a Q1D electron gas was theoretically studied later on by Lee and Spector [6.42]. Further, they investigated momentum relaxation rates for scattering of carriers by ionized impurities considering screening of the impurity potential in a cylindrical wire system. The momentum relaxation rate was found to reduce due to screening effects. Das Sarma and Lai [7.43] also studied the dielectric response function of a 2D electron gas in QWR. They derived a nonsingular screening function appropriate for the investigation of dc transport. Carrier interaction with polar optic phonon was reported [6.44] to be a major scattering mechanism producing hot-electron effects. Riddoch and Ridley [6.45] developed analytical expressions for the scattering rate due to the deformation potential interaction of 1D electrons using MCA. They reported numerical results for polar optic mode of scattering. Their model showed that the scattering and the momentum relaxation rates were found to be significantly enhanced.
over the bulk, the threshold of emission being very abrupt. A similar expression was also provided by Lee and Vassell [6.41] for the relaxation rate for POP scattering of 1D electrons using MCA. Total scattering rate and the transition probability for unscreened electron - POP interaction in 1D system was developed by Leburton [6.46] without considering MCA. We have, however, used Leburton's expression for the scattering rate for polar optic interaction in this chapter to study the one-dimensional hot electron ac mobility in GaAs quantum wires.

Leburton [6.47] studied the 1D electron optical phonon system using the Boltzmann equation where steady-state nonequilibrium and equilibrium electron distributions were observed. Mickevicius et al. [6.48] suggested a 1D system using Monte Carlo simulation. They predicted that for higher electric fields the electrons reach the optical phonon energy threshold which, due to the intensive spontaneous emission of optical phonons, slows their further gain in energy. It was also reported that the electron mobility decreases with increasing electric field since drift velocity reaches saturation.

Zakhleniuk et al. [6.49] developed a Kinetic theory of a nonequilibrium electron gas in a 1D circular quantum wire interacting with acoustic and polar optical phonons together with elastic interaction with interface roughness for the electron momentum relaxation. Boltzmann Kinetic equation was solved
analytically to get different distribution functions for a 1D electron gas. As an application of their theory they calculated the electric field dependence of electron mobility and average energy for different parameters of the QWR. It was reported that at high lattice temperature the electron mobility was monotonous function of the applied electric field and had its maximum value at intermediate electric fields when the transition from acoustic-phonon limited to optical-phonon limited transport took place.

It appears from the scan of the literature that the high frequency response of hot electrons in QWR at high temperature has not yet been reported considering degeneracy of the carriers. This led the author to take up the present investigation. The model and theory relating to this study will now be sketched out in the following section 6.3. Numerical results and discussions are given in section 6.4.

6.3. MODEL AND THEORY:

The cross-section of the QWR is taken to be a square here, so that the width of each of the two spatial directions in which the electron motion is restricted is the same, equal to L(say). The arm of the square cross-section of the QWR (L) is referred to as the channel width in this thesis. For the system parameters of interest here, the separation between the lowest subband and the next higher subband is found to be at least one order of magnitude
greater than the average electron energy for the highest bias field. Thus inter-subband transitions are not significant and hence, in an infinite barrier approximation, the electrons can be considered to occupy the lowest subband only.

In this preliminary work, we take the distribution function \( f(\tilde{k}) \) to be a drifted Fermi-Dirac:

\[
f(\tilde{k}) = f_0(E) + \frac{\hbar \rho_d k_z}{m^*} \left[ - \frac{\partial f_0}{\partial E} \right]
\]

(6.1)

where \( k_z = \sqrt{2 m E / \hbar^2} \) is the 1D wave vector for energy \( E \), \( \rho_d \) is the drift crystal momentum, \( m \) is the electron effective mass, \( \hbar \) is Planck's constant divided by \( 2\pi \), and \( f_0(E) \) is the Fermi-Dirac distribution function with an electron temperature \( T_e \).

The heated Fermi-Dirac distribution function model employed here is strictly valid when electron-electron interactions dominate in the sharing of energy and momentum. In the bulk material, electron-electron scattering is not dominating because the prevailing ionized impurity scattering is of comparable strength. In 1D systems, the effect of the ionized impurity scattering is suppressed due to modulation doping. But here electron-electron scattering leads to an interchange of particles so that the actual distribution differs from the form given by Eq. 6.1. However, we are not interested in the exact shape of the distribution function. Rather, we wish to determine the macroscopic parameters which involve an average
over the distribution function. Fortunately, these parameters are not much sensitive to the exact nature of the distribution function. In fact, the electron temperature model adopted here does not lead to seriously inaccurate results [6.50]. Our model takes less computing time and is free from the statistical fluctuations of a numerical Monte Carlo simulation. It can thus be used to have a feeling of the effects of the changes of various system parameters on the ac mobility. Computationally intensive numerical methods can be applied to analyse the experimental data on 1D ac mobility when they appear in the literature.

In our model, the electron energy loss via the longitudinal optic (LO) phonons and the momentum losses via LO, ionized impurity, and acoustic modes of scattering are incorporated. Scattering rates due to polar coupling with LO phonons can be had from chapter 2[vide Eq.2.41]. The momentum relaxation rates for acoustic and background impurity interactions are also found in chapter 2[vide Eqs. 2.32 and 2.34, respectively].

The electric field applied along the axis of the QWR is assumed to consist of a steady part $F_0$ and a small-signal component with amplitude $F_1$ and angular frequency $\omega$. Both $T_e$ and $\rho_d$ will have similar components with alternating ones generally differing in phase. So we can write:

$$F = F_0 + F_1 \sin \omega t$$

(6.2)
The energy and momentum balance equations obeyed by the carriers are:

\[
\frac{e p_d F}{m} + \frac{dE}{dt} = \frac{dp}{dt} \langle E \rangle, \tag{6.5}
\]

and

\[
\alpha F + \frac{dp}{dt} = \frac{dp_d}{dt} \tag{6.6}
\]

where \(- \frac{dE}{dt}\) and \(- \frac{dp}{dt}\) represent, respectively, the average energy and momentum loss rates due to scatterings, and \(\langle E \rangle\) denotes the average energy of an electron with charge \(e\).

The expression for \(\langle \frac{dE}{dt} \rangle\) and \(\langle \frac{dp}{dt} \rangle\) are:

\[
\langle \frac{dE}{dt} \rangle = A \left[ \int_{0}^{\infty} \frac{1}{\tau} f_o (E) \left[ 1 - f_o (E + \hbar \omega_0) \right] E^{-1/2} dE \right. \\
- \left. \int_{0}^{\infty} \frac{1}{\tau} f_o (E) \left[ 1 - f_o (E - \hbar \omega_0) \right] E^{-1/2} dE \right] \tag{6.7}
\]

\[
\langle \frac{dp}{dt} \rangle = B \left[ \int_{0}^{\infty} \frac{a}{\tau} f_o (E) \left[ 1 - f_o (E) \right] \left[ 1 - f_o (E + \hbar \omega_0) \right] dE \right.
- \left. \int_{0}^{\infty} \frac{a}{\tau} f_o (E) \left[ 1 - f_o (E - \hbar \omega_0) \right] dE \right] \tag{6.7}
\]
\[ \int_{0}^{\infty} \frac{dE}{h\omega_{0}^{1D}} \left[ f_{0}(E) \left[ 1 - f_{0}(E) \right] \left[ 1 - f_{0}(E - \hbar\omega) \right] \right] \]

\[ - C \int_{0}^{\infty} f_{0}(E) E^{-1/2} dE - D \int_{0}^{\infty} f_{0}(E) E^{-3/2} dE \]  

(6.8)

where \( A = \left( \frac{\sqrt{2m\omega_{0}}}{\pi n_{1D}} \right) \), \( B = \frac{2\pi_{d}}{(\pi n_{1D} k_{B} T_{e})} \), \( C = \left( \frac{k_{z}}{\pi n_{1D}^{\tau \text{ac.SQL}}} \right) \), and \( D = \frac{\hbar^{2} k_{z}^{3}}{(\pi \frac{2m}{n_{1D}^{\tau \text{imp.SQL}}})} \).

Here \( k_{B} \) is Boltzmann's constant, \( \omega_{0} \) is the LO phonon angular frequency, \( q_{o}^{a, e} \) and \( q_{1D}^{a, e} \) are the LO phonon wave vectors for the absorption and the emission processes, respectively, and \( 1/\tau_{1D}^{a, e} \) are the scattering rates for LO phonon absorption and emission, respectively, for the 1D system. The expressions for \( q_{1D}^{a, e} \) and \( \tau_{1D}^{a, e} \) can be found in Ref. 6.46. \( \tau_{\text{ac.SQL}}^{\tau} \) and \( \tau_{\text{imp.SQL}}^{\tau} \) are, respectively, the momentum relaxation times for deformation potential acoustic and ionized impurity scattering under the size quantum limit (SQL). Expressions for \( \tau_{\text{ac.SQL}}^{\tau} \) and \( \tau_{\text{imp.SQL}}^{\tau} \) are given in chapter 2 [vide Eqs. 2.32 and 2.34, respectively].

Note that the quantity \( C \) is independent of \( k_{z} \) (and hence \( E \)), since \( \tau_{\text{ac.SQL}}^{\tau} \) is proportional to \( k_{z} \) [6.41]. Also, \( \tau_{\text{imp.SQL}}^{\tau} \) is approximately proportional to \( k_{z}^{3} \) [6.41], the value of \( k_{z} \) in the
slowly varying terms involving Bessel functions being replaced by its average value. So the quantity D is also nearly independent of \( k_z \).

In Eqs. (6.5) and (6.6), we insert Eqs. (6.2-6.4), retain terms up to the first order in the small-signal parts, and equate the steady parts and the coefficients of \( \sin \omega t \) and \( \cos \omega t \) on the two sides of the final equations. We thus obtain:

\[
F_0 \rho_0 = h_1 (T_0), \quad (6.9)
\]

\[
F_0 / \rho_0 = h_2 (T_0), \quad (6.10)
\]

\[
\left[ \frac{F_0}{\rho_0} \right] \left[ \frac{\rho_1}{F_1} \right] - b_3 (T_0) \left[ \frac{T_1}{F_1} \right] = -1, \quad (6.11)
\]

and

\[
\left[ \frac{\rho_1}{F_1} \right] h_4 (T_0) + h_5 (T_0) \left[ \frac{T_1}{F_1} \right] = 1. \quad (6.12)
\]

In the above expressions, \( \rho_1 = \rho_{1r} + j \rho_{1i} \), \( T_1 = T_{1r} + j T_{1i} \) with \( j^2 = -1 \), and the functions \( h_i (T_0) \) \((i = 1-5)\) are determined by the scattering mechanisms. The explicit expressions for \( h_i \)'s are given in Appendix C.

For a given electric field \( F_0 \), \( \rho_0 \) and \( T_0 \) are solved from Eqs. (6.9) and (6.10). Then \( \rho_1 / F_1 \) and \( T_1 / F_1 \) can be found using the Eqs. (6.11) and (6.12).

The dc mobility \( \mu_{dc} \), the small signal ac mobility \( \mu_{ac} \), and the phase lag \( \phi \) of the alternating current behind the applied electric field are given by
6.4. NUMERICAL RESULTS AND DISCUSSIONS:

Calculations are done here for a QWR with the system parameters of GaAs given in Table 3.1.

To be specific about the domain of our work, we find that at the lattice temperature of 77 K, as $F_0$ changes from 0.5 to $1 \times 10^5$ V/m, $T_0$ changes from 138 to 218 K. At a lattice temperature of 300 K, the corresponding variation of $T_0$ is from 310 to 332 K. Allowing $|T_1/T_0| < 0.1$ for the small-signal analysis to hold, we estimate that $F_0 \approx 0.2 \times 10^5$ V/m.

Fig. 6.1 shows the variation of $\mu_{ac}/\mu_{dc}$ with the frequency of the applied electric field for a typical dc bias field of $10^5$ V/m. The curves are obtained with channel width $L = 10$ nm, a 1D carrier concentration of $n_{1D} = 10^8$ m$^{-1}$, and a background ionized impurity concentration of $n_{bi} = 6 \times 10^{21}$ m$^{-3}$. The values of $\mu_{dc}$ are obtained as 1.84 and 0.903 m$^2/(V \cdot s)$ at 77K and 300K, respectively. At lower frequencies, the electric field is practically constant between two successive collisions, forcing
the ac mobility to remain constant. At high frequencies, however, the field changes appreciably between successive collisions, thereby decreasing $\mu_{ac}$. The 3dB cutoff frequency where $\mu_{ac}$ falls to 0.707 of its low-frequency value, is found to be 340GHz for 77K and 360GHz for 300K.

Fig. 6.1: Variation of $\mu_{ac}/\mu_{dc}$ with frequency of the applied electric field for lattice temperatures of 77K and 300K with $F_o = 10^5$V/m, $L = 10\text{mm}$, $n_{1D} = 10^8$/m, and $n_{bi} = 6 \times 10^{21}$m$^{-3}$.

The dependence of phase angle $\phi$ with the frequency of the applied electric field is shown in the Fig. 6.2. The curves are obtained with the parameters of Fig. 6.1. The phase angle $\phi$ is found to increase significantly beyond 10GHz and is higher at 77K than at 300K due to reduced scattering at 77K.
Fig. 6.2: Plot of $\phi$ with the frequency of the applied electric field with the parameters of Fig. 6.1.

Fig. 6.3 gives the variation of $\mu_{ac}$ and $\phi$ with $n_{1D}$ at 77K and 300K at a frequency of 200GHz which is sufficiently high for

Fig. 6.3: Variation of $\mu_{ac}$ and $\phi$ with $n_{1D}$ for a frequency of 200GHz. The other parameters are the same as in Fig. 6.1.
a departure from low-frequency behaviour, the other parameters being the same as in Fig. 6.1. Both $\mu_{ac}$ and $\phi$ generally increase with $n_{1D}$. This is because of the weakening of scattering at higher $n_{1D}$ due to the upward shift of the Fermi level [6.41, 6.46].

The variation of $\mu_{ac}$ and $\phi$ with channel width $L$ at 77K and 300K at a frequency of 200GHz is depicted in Fig. 6.4, the other parameters remaining the same as in Fig. 6.1. Both $\mu_{ac}$ and $\phi$ are found to increase with increasing $L$. The weakening of scattering at higher channel width [6.41, 6.46] accounts for this behaviour.

Fig. 6.5 depicts the channel width dependence of the cutoff frequency $f_{3dB}$ for 77K and 300 K, the other parameters remaining the same as in Fig. 6.1. $f_{3dB}$ is found to decrease with increasing $L$, reflecting that the fall of $\mu_{ac}$ with frequency is sharper at a greater value of $L$. The values of $f_{3dB}$ are found to be higher at 300K than at 77 K.
Fig. 6.5: Variation of $f_{3dB}$ with $L$ with the parameters of Fig. 6.1.

Fig. 6.6 shows the plot of $f_{3dB}$ versus $F_0$. The cutoff frequency increases with the bias field for both 77K and 300K and is found to be higher at 300K than at 77K.

Fig. 6.6: Plot of $f_{3dB}$ versus dc bias field $F_0$. The other parameters are the same as in Fig. 6.1.
The dependence of $f_{3dB}$ on $n_{1D}$ at lattice temperatures of 77 and 300K is depicted in Fig. 6.7. $f_{3dB}$ decreases as $n_{1D}$ increases from 6 to $8 \times 10^7$/cm. But it increases in the range of $n_{1D} = 8$ to $10 \times 10^7$/cm. This is due to the effects of combined scattering processes and upward shift of the Fermi level($E_F$) at higher $n_{1D}$ [6.41, 6.46].

Fig. 6.7: Variation of $f_{3dB}$ with $n_{1D}$ at lattice temperatures of 77 and 300K. The other parameters are the same as in Fig. 6.1.

In chapter 3 (vide Figs. 3.10 and 3.11) it has been observed that the high-frequency response characteristics of 2D hot electron gas are altered when hot phonons are included in the calculations. Kabasi et al.[6.2] reported that the carrier energy and momentum loss rates which offer a fundamental insight into the carrier-phonon interactions, are slowed down in 1D structures considerably when hot phonons are considered. The reduction factor of the total energy-loss rate is 4.4 for $L = 10\,\text{nm}$ at $T = 100\,\text{K}$. The corresponding value for the net momentum loss rate is 2.3. Hence we have studied the high-frequency
response incorporating hot phonons in GaAs QWR along the same line as detailed in chapter 3 for the 2D systems. The variation of ac mobility with frequency including the influence of hot phonons is found to have the same nature as that reported without incorporating hot phonons excepting 5% enhancement in magnitude. The nature of variation and extent of rise of $f_{3dB}$ is again about 25% at 300K just like 2D systems. Thus the effect of hot phonons is almost the same as that obtained for the 2D systems.

The conclusion of this study is given in chapter 8.

REFERENCES:


6.24 E. M. Conwell: "High Field Transport in Semiconductors"


