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Estimation of various scattering parameters and 2-DEG mobilities from electron mobility calculations in the three conduction bands Γ, L and X of gallium arsenide

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Abstract. The electron drift mobility in Γ conduction band of GaAs has been calculated before, but for the first time, we have made attempts to estimate the electron mobilities in higher energy L and X minima. We have also calculated the value of mobility of two-dimensional electron gas needed to predict hetero-structure device characteristics using GaAs. Best scattering parameters have been derived by close comparison between experimental and theoretical mobilities. Room temperature electron mobilities in Γ, L and X valleys are found to be nearly 9094, 945 and 247 cm^2/V-s respectively. For the above valleys, the electron masses, deformation potentials and polar phonon temperatures have been determined to be (0.067, 0.22, 0.39m_0), (8.5, 9.5, 6.5 eV), and (416, 382, 542 K) as best values, respectively. The 2-DEG electron mobility in Γ minimum increases to 1.54×10^6 from 1.59×10^5 cm^2/V-s (for impurity concentration of 10^{14} cm^{-3}) at 10 K. Similarly, the 2-DEG electron mobility values in L and X minima are estimated to be 2.28×10^5 and 1.44×10^5 cm^2/V-s at 10 K, which are about ∼4.5 and ∼3.9 times higher than normal value with impurity scattering present.

Keywords. GaAs; scattering; mobilities in Γ, L and X valleys; effective masses; deformation potential; impurity compensation and 2-DEG.

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1. Introduction

In recent years, scientists started showing considerable interest towards the study and use of compound semiconductors. GaAs is particularly useful in high frequency optoelectronic and microwave devices [1]. Electron transport at high electric fields and temperatures is dominated by the complex conduction-band structure well above the lowest band edge. Further, electronic properties of ternary and quaternary compounds using GaAs as one of the binary compounds are largely influenced by the electron occupation of higher energy conduction band minima at L and X.

To predict the device performance, it is imperative to know the scattering parameters of not only the lowest band Γ minimum but also of higher energy L and X minima. From this point of view, the calculation of mobilities in higher lying L and X minima are extremely important. Obviously, one now has a wider selection of band structures, as compared to column IV semiconductors alone [2].

2. Analysis

In the analysis, the following simplifying assumptions are made: (a) Each electron scattering process is described by a relaxation time $\tau(y)$ which depends upon the electron energy y in $K_{\mathrm{B}}T$, where K_{B} is the Boltzmann's constant, (b) the electrons are assumed to be scattered in a parabolic band. This allows us to use simpler formulations for the various scattering events, (c) for each scattering process, an average relaxation time $\langle\tau_i\rangle$ is calculated from the equation

$$\langle\tau_i\rangle = \frac{4}{3\sqrt{\pi}} \int_0^{\infty} \tau_i(y) y^{3/2} \exp(-y)\mathrm{d}y. \qquad (1)$$

The electron mobility is then calculated from the equation

$$\mu_i = q\langle\tau_{\mathrm{I}}\rangle/m^*, \qquad (2)$$

where q is the electronic charge and m^* is the electron effective mass in the minima involved. As an approximation, various scattering mechanisms have been considered independent of each other. The resultant mobility is then defined by Mattheissien rule, i.e.

$$\mu^{-1} = \sum_i \mu_i^{-1}. \qquad (3)$$

Although these assumptions are not *a priori* strictly valid, calculations based on these assumptions are in good agreement with experiment. The following scattering mechanisms have been considered.

2.1 *Ionized impurity scattering*

The electrons are scattered by a charged shallow impurity in the semiconductor. The ionized impurity scattering is described by the Brooks Herring equation which takes into account screening of the scattering potential. Using the relaxation time [3] and eqs (1) and (2), one obtains the ionized impurity scattering mobility μ_{I}, which reads as

$$\mu_{\mathrm{I}} = \frac{3.28 * 10^{15} \varepsilon_{\mathrm{s}}^2 T^{3/2}}{N_{\mathrm{I}}(m^*/m_0)^{1/2}\left[\ln(b+1) - \frac{b}{b+1}\right]}\ \mathrm{cm}^2/\mathrm{V\text{-}s} \qquad (4)$$

with $b = [1.29{*}10^{14}(m^*/m_0)\varepsilon_{\mathrm{s}}T^2]/n^*$, $n^* = n + [(n+N_{\mathrm{A}})\{(N_{\mathrm{D}}-N_{\mathrm{A}}-n)/N_{\mathrm{D}}\}]/\mathrm{cm}^3$, and $n = (N_{\mathrm{D}} - N_{\mathrm{A}})/\mathrm{cm}^3$ where n^* is the effective screening density and m_0 the free electron mass.

Conwell and Weisskpof [4] also suggested that the electron drift mobility due to ionized center scattering is given by

$$\mu_{\mathrm{C}} = \frac{CT^{3/2}N_{\mathrm{I}}^{-1}}{\ln[1+DN_{\mathrm{I}}^{-2/3}T^2]}\mathrm{cm}^2/\mathrm{V\text{-}s}, \tag{5}$$

where $C = [64\pi^{1/2}(\varepsilon_{\mathrm{s}}\varepsilon_0)^2(2K_{\mathrm{B}})^{3/2}]/Z_1^2q^3(m^*)^{1/2}$ and $D = (12\pi(\varepsilon_{\mathrm{s}}\varepsilon_0)K_{\mathrm{B}}/Z_1q^2)^2$ and Z_1 the degree of ionization is taken to be unity. Comparing eqs (5) and (5) reveals that both formulas are very similar except that the coefficient inside the logarithmic term is slightly different. It is interesting to note that both formulas predict the same temperature dependence for the ionized impurity scattering mobility.

2.2 *Deformation potential scattering*

The change of lattice spacing with respect to its equilibrium position due to lattice vibrations results in deformation potential. An acoustical wave may induce a change in the spacing of neighboring atoms in a semiconductor. This change in atomic spacing could result in the fluctuation of energy band gap locally on an atomic scale and is known as the deformation potential. Using the relaxation time for deformation potential scattering based on the theory of Bardeen and Shockley [5] as given by Wolfe *et al* [6] similarly gives

$$\mu_{\mathrm{DP}} = \frac{3.17*10^{-5}*d*u^2}{(m^*/m_0)^{5/2}E_{c_1}^2T^{3/2}}\ \mathrm{cm}^2/\mathrm{V\text{-}s}, \tag{6}$$

where d and u being the material density and sound velocity, respectively and E_{c_1} is the acoustic deformation potential in eV.

2.3 *Piezoelectric scattering*

For polar semiconductors such as III–V, the bonds are partially ionic and the unit cell does not possess inversion symmetry. In crystals having no inversion symmetry, the displacement of the atoms associated with the acoustic waves produces an electric field. This effect is usually referred to as piezoelectric effect. As a result, charged carriers may be scattered by longitudinal-mode acoustical phonons and cause piezoelectric scattering. The relaxation time for piezoelectric scattering as determined by Zook [7] similarly gives the expression

$$\mu_{\mathrm{PE}} = 43.0\left(\frac{300}{T}\right)^{1/2}\frac{\varepsilon_0^2}{(m^*/m_0)^{3/2}}\ \mathrm{cm}^2/\mathrm{V\text{-}s}. \tag{7}$$

Since the contribution of this scattering mechanism to the resultant mobility is found to be appreciably smaller than that due to the other scattering processes considered here, the uncertainty in the material parameters involved results in a negligibly small error.

2.4 *Inter- and intra-valley scatterings*

For multivalley conduction band minima at L and X points in Brillouin zone, intra-valley and inter-valley scatterings (i.e., scattering within a single conduction band minimum L or X and between L and X minima, respectively) near room temperature is usually accompanied by absorption or emission of a longitudinal-mode acoustical phonons. Fawcett and Paige [9] have given the expression for the scattering rate for scattering from state k in valley i to a state in valley j. In the approximation $E \cong 3/2K_{\mathrm{B}}T$, we similarly get

$$\mu_{iv} = \mu_{ac}\left(\frac{1}{\alpha}\right)\left(\frac{T}{T_c}\right)^{3/2}\frac{4\sqrt{2}}{\sqrt{3}}\frac{1}{(Z_j-1)}r^{-1}$$

with

$$r = \left[\frac{\{T/T_c + 2/3 + (\Delta_i - \Delta_j)/K_{\mathrm{B}}T\}^{1/2}}{(\mathrm{e}^{T_c/T}-1)} + B\right] \tag{8}$$

$$B = \left[\frac{\{T/T_c - 2/3 + (\Delta_i - \Delta_j)/K_{\mathrm{B}}T\}^{1/2}}{(1-\mathrm{e}^{-T_c/T})}\right] \quad \text{or } 0 \tag{9}$$

for $T/T_c \leq 2/3 + (\Delta_i - \Delta_j)/K_{\mathrm{B}}T$ and

$$\alpha = \frac{2D_{ij}^2 u^2}{E_{c_1}^2 \omega_l^2}. \tag{10}$$

The energy separation $(\Delta_i - \Delta_j)$ between the two minima should be set equal to zero for intra-valley scatterings, since they will be at the same energy. T_c is the Debye temperature and ω_l is the phonon frequency. For inter-valley scatterings, $(Z_j - 1)$ is replaced by Z_J. We have taken $Z_j = 6$ for X and 4 for L with sub-band gap $\Delta E_{\mathrm{LX}} = 0.20$ eV.

2.5 *Polar optical phonon scattering*

The phonon characterizing the vibration in polarizable materials is known as polar phonon. The theoretical expression of electron mobility derived by Fortini [10] is given by the expression

$$\mu_{\mathrm{po}} = 25.4\frac{T^{1/2}}{T_c}\left(\frac{1}{\varepsilon}-\frac{1}{\varepsilon_{\mathrm{s}}}\right)^{-1}\left(\frac{m_0}{m^*}\right)^{3/2}(\mathrm{e}^Z - 1)G(Z)\ \mathrm{cm}^2/\mathrm{V\text{-}s}. \tag{11}$$

Here T_c is the polar phonon Debye temperature and $Z = T_c/T$. $G(Z)$ is the quantity defined by Howarth and Sondheimer [11]. ε_{s} is the static and ε the high frequency dielectric constant.

3. Modeling of $\mu(T)$

The temperature variation of $\mu_{\Gamma,\mathrm{L,X}}$ reported here have been matched with those required to explain the experimental mobility data for GaAlAs alloys [12]. The values listed in table 1[1] are the matched values for best fitting.

3.1 Γ *valley*

The ionized impurity scattering is the dominant scattering mechanism in low temperature region as seen from figure 1[2]. Room temperature mobility is found to be nearly 9094 cm^2/V-s. Near liquid nitrogen temperature, it is about 18,000 cm^2/V-s. If ionized impurity scattering is removed in figure 1, then the 10 K mobility will shoot up to 1.54×10^6 cm^2/V-s which is about 10 times higher than the value shown in the figure. The 2-DEG electrons in GaAs used in hetero-structure devices will have much higher mobilities, a parameter of great interest for high frequency devices.

3.2 *For L valleys*

Since GaSb belongs to III–V group, parameters of this binary compound are used to calculate the mobility for L valleys. Although Γ valley is the minimum conduction band in GaSb, energy separation between Γ and L valleys is very small and therefore at room temperature nearly all the electrons reside in the L valley of GaSb due to higher density of states. Later in the same model, parameters pertinent to GaAs have been used to assess L mobility values in GaAs. Ionized impurity, deformation potential, polar optical phonon and piezoelectric mobilities are considered as observed in figure 2. L minima mobility in GaAs is then found to be 945 cm^2/V-s. The 2-DEG electron mobility in L minima increases to 2.28×10^5 cm^2/V-s, an increase by a factor of $\sim$4.5 at 10 K.

3.3 *For X valleys*

Similar treatment for the calculation of mobility for X valleys is applied as in the case of calculation of mobility for L valleys. Here we took the data of the binary compound GaP, where the X valleys have minimum conduction band energy. GaP should predict the behavior similar to the X valleys of GaAs. After testing the model on GaP, parameter values relevant to GaAs were plugged in the program. Ionized impurity, deformation potential, polar optical phonon and piezoelectric mobilities are considered. As seen from figure 3, room temperature mobility is found to be 247 cm^2/V-s. The 2-DEG electron mobility in X minima has a value of 1.44×10^5 cm^2/V-s, an increase by a factor of $\sim$3.9 at 10 K.

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[1] For table 1, see http://www.ias.ac.in/pramana/v69/p687/supplement.pdf

[2] For figures 1–4, see http://www.ias.ac.in/pramana/v69/p687/supplement.pdf

The X mobility was measured on GaAs under pressure to invert the band structure in order to have direct assess to X electrons for measurements (figure 4). The lower and higher temperatures are limited by the cooling arrangement of pressure system and it is not possible to go further down or above room temperature with the system used [16]. Each scattering mechanism has a different temperature dependence and the values listed in table 1 represent their best combination. Changing any one of them will deteriorate the fit in some temperature region. The margin on X valley mass and intra-valley deformation potential are $(0.39\pm0.01)m_0$ and (6.5 ± 0.1) eV, respectively.

4. Results and conclusions

Various parameters needed to fit the experimental data have already been tabulated in table 1. This data on GaAs should be very useful for optoelectronic devices working at high fields and temperatures and also for ternary and quaternary devices. The 2-DEG mobility should also be helpful to hetero-structure device designers. The room temperature mobility in Γ minimum was found to be $\sim$9094 cm^2/V-s. For L valleys, the mobility is found to be $\sim$947 cm^2/V-s with single valley electron effective mass $= 0.22m_0$ and deformation potential = 8.5 eV. For X valleys, an accurate comparison between theoretical and experimental mobilities have been shown. A single valley density of state effective mass $0.39m_0$ is required to fit experimental data. Room temperature mobility is found to be 217 cm^2/V-s. The 2-DEG mobilities at low temperatures increase considerably over the values with impurity scattering present.

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Supplementary pages

Table 1. Summary of various parameters fitted with experimental mobility data describing the lower conduction band minima of GaAs [1,7,11–16].

Parameter	Γ valley	L valley	X valley
Single valley density of state effective mass (m^*)	$0.067m_0$	$0.22m_0$	$0.39m_0$
No. of equivalent minima (Z_j)	1	4	6
Density (d)	5.32 g/cc	5.23 g/cc	2.33 g/cc
Acoustic speed (u)	$5.24*10^5$ cm/s	$3.63*10^5$cm/s	$6.82*10^5$cm/s
Intra-valley deformation potential (E_{c1})	8.5 eV	9.5 eV	6.5 eV
Static dielectric constant (ε_s)	12.91 F/cm	15.98 F/cm	11.8 F/cm
High frequency dielectric constant (ε)	10.92 F/cm	–	–
Polar phonon Debye temperature (T_c)	416 K	382 K (346 for GaSb)	542 K (580 for GaP)
Inter-valley deformation potential field (D_{ij})	–	$3*10^8$ eV/cm	$3*10^8$ eV/cm
Non-polar optical phonon deformation potential (E_{npo})	–	6.2 eV	6.4 eV
Ionized impurity (N_I)	10^{14}/cm^3	10^{14}/cm^3	10^{14}/cm^3

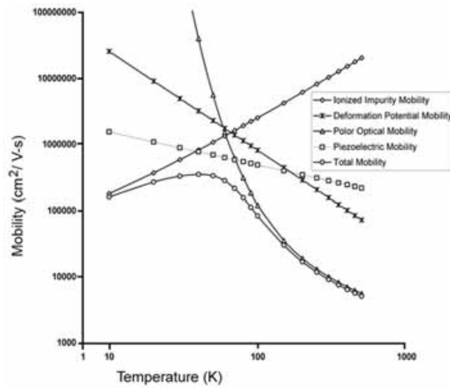

Figure 1. Temperature vs. mobility for Γ electrons in GaAs.

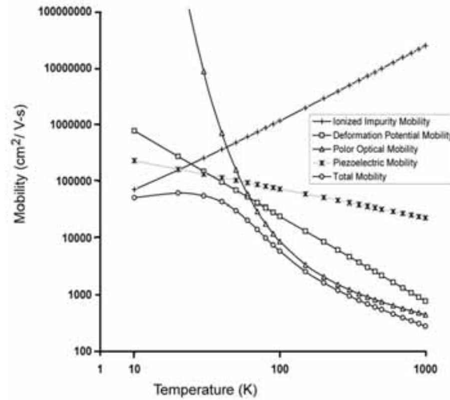

Figure 2. Temperature vs. mobility for L electrons in GaAs.

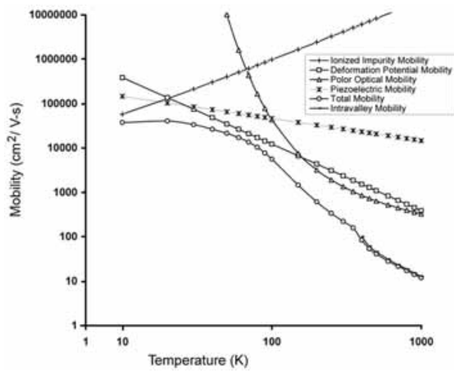

Figure 3. Temperature vs. mobility for X electrons in GaAs.

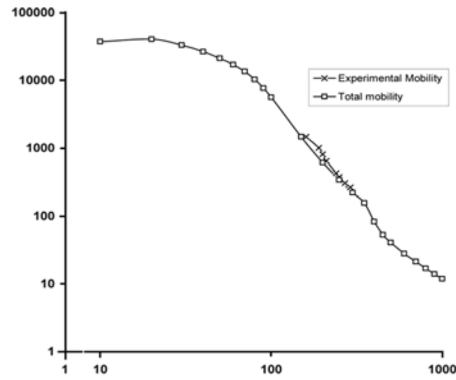

Figure 4. Comparison of experimental and resultant mobility for X electrons in GaAs.