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Effect of Screening on Piezoelectric Scattering Rates of Free Electrons in 2DEG

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Abstract: ***The piezoelectric scattering rate of free electrons is investigated in a degenerate two-dimensional electron gas (2DEG) formed in semiconductor interface giving due account to the effect of screening of the free carriers and the true phonon distribution which are indeed dominant features at low lattice temperatures. Numerical calculations are made to observe the effect in GaAs surface layer.***

Keywords: 2DEG, Piezoelectric, Phonon, Scattering, Screening

1. Introduction

The study of the transport properties of III-V hetero-interface has drawn considerable attention because of the very high mobility of the two-dimensional electron gas (2DEG) in these systems at low temperature [1]. A triangular quantum well is formed at the AlGaAs/GaAs interface and in the triangular well only the quantum mechanical ground state is populated by free electrons at low lattice temperatures ($T_L < 100\,\mathrm{K}$), making the system one of the best experimental realizations of a 2DEG in nature.

The theoretically calculated transport characteristics in a 2DEG depend on the theoretical models adopted in their calculations. To test the various theoretical predictions about the behavior of the characteristics due to different type of scattering mechanisms, one must know which type of scattering is predominant in a particular material under the prevalent condition of lattice temperature T_L and free carrier concentration N_i.

At low temperatures the free carriers are dominantly scattered by the intravalley acoustic phonon and by impurity ions. The optical and intervalley phonon scattering are important only at high temperatures when an appreciable number of corresponding phonons is excited or in the presence of a high electric field when the non-equilibrium electrons can emit high energy phonons. This apart, the scattering due to surface roughness may also arise because of non-planarity of the semiconductor interface. Of all these, the scattering involving intravalley acoustic phonons is the most important mechanism in controlling the electrical transport at low lattice temperatures ($T_L < 20\,\mathrm{K}$) if the content of the impurity atoms in the system under study is relatively low [2-10]. The free carriers in a covalent crystal interact dominantly only with acoustic phonons through deformation potential. On the other, if a crystal consists of dissimilar atoms such as GaAs, the bonds are partly ionic and the unit cell does not contain a center of symmetry and electrons interact with acoustic phonons due to both deformation potential as well as piezoelectric coupling [6,7,11,12]. Again with the lowering of lattice temperature a number of features arises which are different from those of higher temperatures. These are the non-equipartition energy distribution of phonons, degeneracy of the free carrier ensemble, electrostatic screening of the scattering potential by the electron ensemble etc. Taking all these features into account at a time it is very difficult to study the electrical transport in 2DEG and hence to do the same one has to adopt theoretical model imparting reasonable approximations.

A number of works on the study of electrical transport in 2DEG at low temperatures have already been reported by the present author [9,10,13-15]. Störmer et al. [16] studied Shubnikov-de-Haas oscillations in GaAs-$Ga_xAl_{1-x}As$ hetero-structure around 4.2K and reported the mobility values. Shinba and Nakamura [17] developed a comprehensive theory of phonon limited electron mobility in a degenerate 2DEG at low lattice temperature ($T_L < 50\,\mathrm{K}$). Lei et al [18] have developed a non-Boltzmann theory of the steady state transport using the full phonon distribution at low temperatures and studied the transport characteristics in GaAs-$Ga_xAl_{1-x}As$ heterojunctions. A theory of intravalley acoustic phonon scattering of the free carriers in a non-degenerate 2DEG has been developed by the present author [10] and the zero-field mobility characteristics in Si inversion layers has been determined with the help of Monte Carlo simulation of velocity autocorrelation function.

At low temperatures the Fermi energy of the free electrons in a 2DEG is usually greater than their thermal energy and hence the electron system obeys the degenerate statistics. In degenerate 2DEG the Fermi energy is seen to be much higher than the intravalley acoustic phonon energy and hence the electron-phonon collisions are usually considered to be quasi-elastic. But unlike the traditional practice, the energy distribution of phonons cannot be approximated by the equipartition law of the Bose-Einstein distribution function in view of the low temperature range of interest here. Again with the lowering of lattice temperature the electronic system starts to be degenerate and then the effect of screening of the free carriers may significantly influence the electrical transport [3,19,20]. Thus the phonon-limited electron mobility in a degenerate 2DEG has been studied by the present author considering the true phonon population given by Bose-Einstein distribution function and the effect of screening due to free carriers at low lattice temperatures when the electrons interact only with deformation potential acoustic phonons [13]. In this article the scattering rates of the free electrons for their interaction with piezoelectric acoustic phonons has been calculated in a degenerate 2DEG system at low lattice temperature giving due account to the true phonon population and the effect of screening of the free electrons in the system. The result is then applied to observe the temperature dependence of the piezoelectric scattering rates of free electrons in a degenerate 2DEG formed in GaAs inversion layer.

2. Theory

The conduction electrons of a two dimensional electron gas formed in oxide-semiconductor interface are free to propagate in the x-y plane parallel to the interface but are confined by the potential due to surface electric field E_s in the z-direction perpendicular to the interface. Assuming spherical constant energy surfaces the energy eigen values of the electrons in a surface channel represented by a triangular potential well can be expressed as [5]

$$\epsilon = \epsilon_{\vec{k}} + \epsilon_n = \frac{\hbar^2 k^2}{2m_\parallel^*} + \epsilon_n = \frac{\hbar^2 k_x^2}{2m_1^*} + \frac{\hbar^2 k_y^2}{2m_2^*} + \left[\frac{e^2\hbar^2 E_s^2}{2m_\perp^*}\right]^{1/3} \gamma_n, \quad (1)$$

where $\epsilon_{\vec{k}}$ is the energy of the electron, $\vec{k}$ is the component of the electron wave vector parallel to the interface, $\hbar(= h/2\pi)$ is the Dirac constant and $m_\parallel^* = (m_1^* m_2^*)^{1/2}$ is the effective mass of the electron parallel to the interface; ϵ_n is the energy of the n-th subband, the surface electric field $E_s = eN_i/\varepsilon_d$, e being the electronic charge and ε_d the static dielectric constant of the semiconductor, $m_\perp^*$ is the effective mass perpendicular to the surface, and γ_n are the roots of the equation $A_i(-\gamma_n) = 0$; $A_i(-z)$ being Airy function.

Usually at low temperatures only the lowest subband with $n = 0$ is occupied and the higher subbands do not play any significant role. Hence the *z*-direction can altogether be ignored and the conductor may simply be treated as a two-dimensional system in the *x-y* plane. As such the principal mode of lattice vibrations which can interact with such quantized electrons in a semiconductor inversion layer are two-dimensional acoustic waves. The phonons normal to the layer simply cause mixing of the subbands [3].

The piezoelectric scattering rate of an electron with energy $\epsilon_{\vec{k}}$ in a degenerate 2DEG can be obtained from the perturbation theory as [5,6,7]

$$P_{pz}(\epsilon_{\vec{k}}) = \frac{2\pi}{\hbar}\int_{\theta=0}^{2\pi}\int_{q_1}^{q_2} \frac{s}{(2\pi)^2}\Big[\left|\langle \vec{k}+\vec{q}|H_{pz}'|\vec{k}\rangle\right|^2 \times \{1 - f_0(\vec{k}+\vec{q})\}\delta(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} - \hbar q u_l) + \left|\langle \vec{k}-\vec{q}|H_{pz}'|\vec{k}\rangle\right|^2\{1 - f_0(\vec{k}-\vec{q})\} \times \delta\left(\epsilon_{\vec{k}-\vec{q}} - \epsilon_{\vec{k}} + \hbar q u_l\right)\Big]\, q\, dq\, d\theta. \quad (2)$$

Here the matrix element corresponding to the piezoelectric interaction of the free electrons is anisotropic because of the anisotropy of the piezoelectric tensor. However, the properly averaged squared matrix element can be given as [6,11]

$$\left|\langle \vec{k}\pm\vec{q}|H_{pz}'|\vec{k}\rangle\right|^2 = \left(\frac{e^2\hbar k_m^2 u_l q}{4sd\varepsilon_d k^2}\right) S^2(q)\left(N_q + \frac{1}{2} \pm \frac{1}{2}\right).$$

Here k_m is the piezoelectric coupling constant of the material. The parameter s is the surface area, d the width of the layer of lattice atoms with which the electrons can interact, q the component of the phonon wave vector parallel to interface, u_l the acoustic velocity and N_q is the phonon population. The function $f_0(\vec{k}\pm\vec{q})$ is the probability of occupation of the final state $\vec{k}\pm\vec{q}$ and is given by the Fermi function. The upper and lower sign corresponds respectively to the processes of absorption and emission. The parameters q_1 and q_2 are respectively, the lower and upper limits of q. The screening factor $S(q)$ is defined in the static limit, since the momentum and energy conservation conditions limit the interaction with electrons with long wavelengths only and then in a 2DEG, $S(q)$ can be given as [3,19]

$$S(q) = \frac{q}{q + q_s}, \quad (3)$$

where for degenerate 2DEG

$$q_s = \frac{e^2 m_\parallel^*}{2\pi\varepsilon_d \hbar^2}.$$

In a degenerate 2DEG, as mentioned earlier, the electrons with energy around the Fermi energy $\epsilon_F(= \pi\hbar^2 N_i/n_v m_\parallel^*)$ control the transport. Here n_v is the number of equivalent valleys at the surface. The Fermi energy in degenerate 2DEG is usually seen to be much greater than the acoustic phonon energy. Thus the electron-phonon collisions may be considered to be quasi-elastic in these systems and the phonon energy $\hbar q u_l$ can be neglected in the energy balance equation of electron-phonon interaction. Consequently, the distribution function $f_0(\vec{k}\pm\vec{q})$ can be approximated to the Fermi distribution function $f_0(\vec{k})$. Then integration over θ in Eq.(2) can be carried out yielding

$$P_{pz}(\epsilon_{\vec{k}}) = \frac{e^2 k_m^2 u_l m_\parallel^*}{4\pi\hbar^2 d\varepsilon_d k^3}\left[1 - f_0(\vec{k})\right] \times \int_{q_1}^{q_2} \frac{(2N_q + 1)S^2(q) q\, dq}{[1 - (q/2k)^2]^{1/2}}. \quad (4)$$

At low lattice temperatures the true phonon distribution may be given by the Laurent expansion as [21]

$$N_q(x) = \sum_{m=0}^{\infty} \frac{B_m}{m!} x^{m-1} \quad ; \quad x \le \bar{x}, \qquad \approx 0 \quad ; \quad x > \bar{x}, \quad (5)$$

where $x = \hbar q u_l / k_B T_L$, k_B being the Boltzmann constant. B_m's are Bernoulli numbers and $\bar{x} < 2\pi$. For the practical purpose $\bar{x}$ may be taken to be 3.5.

The lower (q_1) and upper (q_2) limits of the integration in Eq.(4) can be deduced from the energy and momentum conservation equations for an electron making transition from a state $\vec{k}$ to $\vec{k}\pm\vec{q}$ in course of a collision accompanied by either absorption or emission of a phonon. The respective limits for both absorption and emission processes can be approximated to be 0 and $2k$ for the electron-phonon system of interest here. Hence carrying out the integration in Eq.(4) one obtains

$$P_{pz}(\epsilon_{\vec{k}}) = \frac{\mathcal{A}_{pz}}{\epsilon_{\vec{k}}}\lambda\left[1 - f_0(\epsilon_{\vec{k}})\right]\mathcal{F}_m(\epsilon_{\vec{k}}). \quad (6)$$

Here

$$\mathcal{A}_{pz} = \left(\frac{e^2 k_m^2}{16\pi\hbar d\varepsilon_d}\right)\frac{(k_B T_L)^2}{\sqrt{\varepsilon_s}}, \quad \varepsilon_s = \frac{1}{2}m_\parallel^* u_l^2, \quad \lambda = \frac{4\sqrt{\varepsilon_s}}{k_B T_L}.$$

The function $\mathcal{F}_m(\epsilon_{\vec{k}})$ assumes different forms in the different range of electron energy. Thus when the screening effect and true phonon distribution are taken into account $\mathcal{F}_m(\epsilon_{\vec{k}})$ takes the form

$$\mathcal{F}_m(\epsilon_{\vec{k}}) = \sum_{m=0}^{\infty} \frac{2B_{2m}}{(2m)!}\left[\sum_{n=0}^{2m}(-x_s)^n\binom{2m+2}{n} \times\left\{J_{2m-n+1}\left(\frac{1}{x_s}\right) - J_{2m-n+1}\left(\frac{1}{x_s+x_c}\right)\right\} + \sum_{n=2m+1}^{2m+2}(-x_s)^n\binom{2m+2}{n} \times\left\{I_{n-2m-1}\left(\frac{1}{x_s}\right) - I_{n-2m-1}\left(\frac{1}{x_s+x_c}\right)\right\}\right]; \quad \text{for } x_c \le \bar{x},$$

$$= \sum_{m=0}^{\infty} \frac{2B_{2m}}{(2m)!}\left[\sum_{n=0}^{2m}(-x_s)^n\binom{2m+2}{n} \times\left\{J_{2m-n+1}\left(\frac{1}{x_s}\right) - J_{2m-n+1}\left(\frac{1}{x_s+\bar{x}}\right)\right\} + \sum_{n=2m+1}^{2m+2}(-x_s)^n\binom{2m+2}{n} \times\left\{I_{n-2m-1}\left(\frac{1}{x_s}\right) - I_{n-2m-1}\left(\frac{1}{x_s+\bar{x}}\right)\right\}\right] + \sum_{n=0}^{1}(-x_s)^n\binom{3}{n}\left\{J_{2-n}\left(\frac{1}{x_s+\bar{x}}\right) - J_{2-n}\left(\frac{1}{x_s+x_c}\right)\right\} + \sum_{n=2}^{3}(-x_s)^n\binom{3}{n}\left\{I_{n-2}\left(\frac{1}{x_s+\bar{x}}\right) - I_{n-2}\left(\frac{1}{x_s+x_c}\right)\right\}; \quad \text{for } x_c > \bar{x}. \quad (7)$$

Here

$$x_c = \lambda\sqrt{\epsilon_{\vec{k}}}, \quad x_s = \frac{\hbar q_s u_l}{k_B T_L},$$

$$J_p(x) = -\frac{\sqrt{R(x)}}{(p-1)ax^{p-1}} - \frac{(2p-3)b}{2(p-1)a}J_{p-1}(x) - \frac{(p-2)c}{(p-1)a}J_{p-2}(x),$$

$$J_1(x) = \frac{1}{\sqrt{-a}}\sin^{-1}\left(\frac{2a+bx}{x\sqrt{-\Delta}}\right),$$

$$I_p(x) = -\frac{x^{p-1}}{pc}\sqrt{R(x)} - \frac{(2p-1)b}{2pc}I_{p-1}(x) - \frac{(p-1)a}{pc}I_{p-2}(x),$$

$$I_0(x) = \frac{1}{\sqrt{c}}\ln\left[2\sqrt{cR(x)} + 2cx + b\right]; \quad \text{for } x_s < x_c,$$

$$= \frac{-1}{\sqrt{-c}}\sin^{-1}\left(\frac{2cx+b}{\sqrt{-\Delta}}\right); \quad \text{for } x_s > x_c,$$

$$\Delta = 4ac - b^2, \quad R(x) = a + bx + cx^2,$$

$$a = -1, \quad b = 2x_s, \quad c = x_c^2 - x_s^2,$$

$$\binom{m}{n} = \frac{m(m-1)\dots(m-n+1)}{n!}, \quad \binom{m}{0} = 1.$$

When the screening effect is neglected one should put $S(q) = 1$ in Eq.(4) and then considering only true phonon distribution as given in Eq.(5) one obtains $\mathcal{F}_m(\epsilon_{\vec{k}})$ as

$$\mathcal{F}_m(\epsilon_{\vec{k}}) = \pi + \sum_{m=1}^{\infty}\frac{\pi B_{2m}(2m-1)!!}{(2m)!\,(2m)!!}x_c^{2m}; \quad \text{for } x_c \le \bar{x},$$

$$= \sum_{m=0}^{\infty}\frac{2B_{2m}}{(2m)!}\mathcal{C}_{2m}(\bar{\theta})x_c^{2m} + x_c\cos\bar{\theta}; \quad \text{for } x_c > \bar{x}. \quad (8)$$

Here

$$\mathcal{C}_p(\theta) = -\frac{\sin^{p-1}\theta\cos\theta}{p} + \frac{p-1}{p}\mathcal{C}_{p-2}(\theta),$$

$$\mathcal{C}_0(\theta) = \theta, \quad \bar{\theta} = \sin^{-1}(\bar{x}/x_c).$$

Under the high temperature condition when the equipartition law holds good then if one considers the screening effect the function $\mathcal{F}_m(\epsilon_{\vec{k}})$ takes the form as

$$\mathcal{F}_m(\epsilon_{\vec{k}}) = 2\left[J_1\left(\frac{1}{x_s}\right) - J_1\left(\frac{1}{x_s+x_c}\right)\right] - 4x_s\left[I_0\left(\frac{1}{x_s}\right) - I_0\left(\frac{1}{x_s+x_c}\right)\right] + 2x_s^2\left[I_1\left(\frac{1}{x_s}\right) - I_1\left(\frac{1}{x_s+x_c}\right)\right], \quad (9)$$

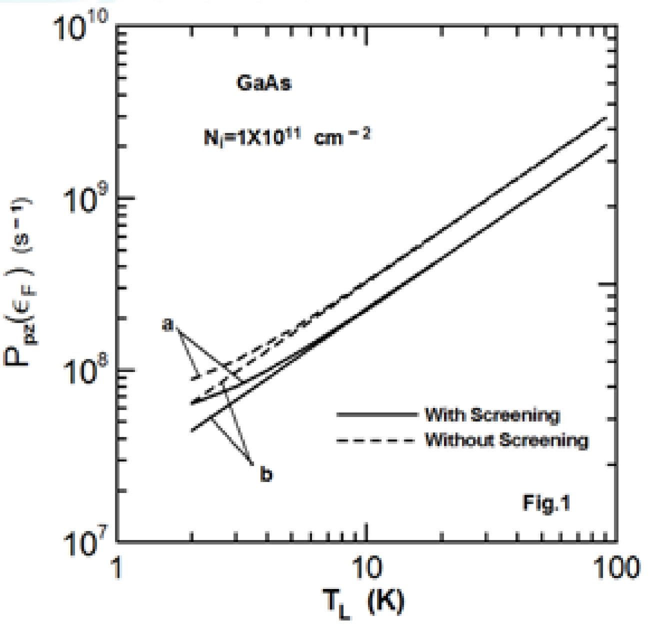
and, under the same condition if the screening effect is neglected

$$\mathcal{F}_m(\epsilon_{\vec{k}}) = \pi. \quad (10)$$

3. Result and Discussion

It turns out from Eqs. (7), (8), (9) and (10) that when the free-carrier screening factor and the full phonon distribution is taken into account, the piezoelectric scattering rates of the free electron in a degenerate 2DEG depend upon carrier energy and lattice temperature in a quite complex manner. For an application of the above formulation, sample of GaAs is considered with the material parameter values [11]: $k_m = 0.052$, $u_l = 5.2\times10^3$ m s^{-1}, $\varepsilon_d = 13.5$, effective mass $m^* = 0.067m_0$, m_0 being the free electron mass. At low temperatures, considering the electrical quantum limit the electrons are populated in the lowest subband [5] when the layer thickness $d = (\hbar^2\varepsilon_d/2m_\perp^* e^2 N_i)^{1/3}\gamma_0$. For GaAs, $m_\parallel^* = m_\perp^* = m^*$.

The effect of screening on the piezoelectric scattering rates of the electrons with Fermi energy in a degenerate 2DEG controlled by the piezoelectric acoustic phonons at different temperatures are plotted in Figure1 and Figure2 for two different carrier concentrations.



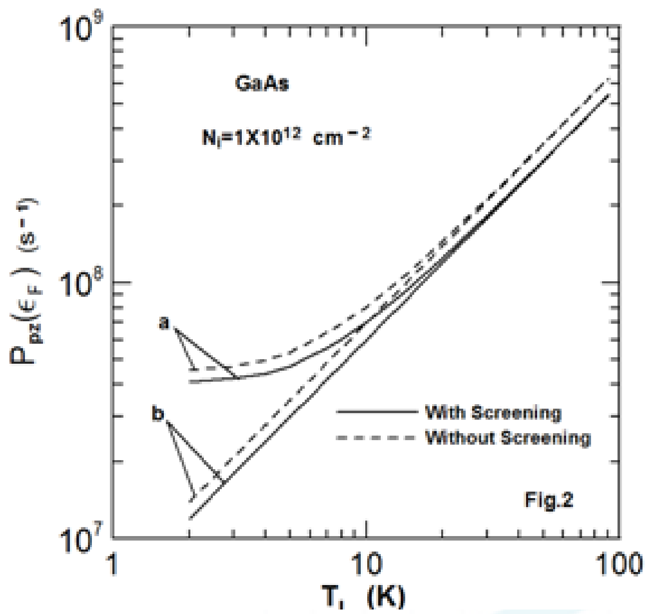


Figure 1 & **Figure 2:** Dependence of the piezoelectric scattering rates of free electrons with Fermi energy upon the lattice temperatures for 2DEG layer of GaAs. Curves marked a and b indicate respectively the contribution from the full phonon spectrum and its equipartition approximation.

Figures show that the scattering rates obtained here giving due account to the screening effect of the free carriers are smaller whether the full phonon distribution is considered or not. Again it is observed that the consideration of the full phonon distribution plays a significant role in estimating the scattering rates at lower temperatures and higher carrier concentrations. It is seen from Eq.(3) that the screening factor for 2DEG system is independent of temperature and as such the qualitative change in the shape of the scattering characteristics is absent whether the equipartition law is taken under consideration or not. But an appreciable deviation in the characteristics is seen particularly at low lattice temperatures.

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