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Effect of Screening on Acoustic Phonon Limited Electron Mobility in Quantized Surface Layer in Semiconductor

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***Abstract*— Intravalley acoustic phonon scattering rates of electrons are calculated in a degenerate two-dimensional electron gas (2DEG) formed in semiconductor interfaces giving due account to the effect of screening of the free carriers and the true phonon distribution which are the dominant characteristics at low lattice temperatures. The results of the scattering rates and the subsequent zero-field electron mobility are estimated for an n-channel (100) oriented Si inversion layer. The results are compared with the available experimental and other theoretical results.**

***Index Terms*— Electron Mobility, Quantized Surface, Screening, Semiconductor.**

I. Introduction

The inversion and/or accumulation layers can form near semiconductor interfaces under the application of sufficiently strong electric field as it is observed in the metal-oxide-silicon (MOS) devices. The study of the electrical transport properties of the system of two-dimensional electron gas (2DEG) formed in such layers has drawn a considerable attention from both the fundamental and technological points of view.

The transitions of a free carrier in surface layer are induced by different scattering sources and their relative importance is determined by the lattice temperature T_L and free carrier concentration. At low temperatures the free carriers are dominantly scattered by the intravalley acoustic phonon and by impurity ions. The optical and intervalley phonon scattering can be 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 electron-phonon scattering is an intrinsic process and the scattering involving intravalley acoustic phonons is the most important mechanism in controlling the electrical transport at low lattice temperatures ($T_L < 20$ K) if the content of the impurity atoms in the system under study is relatively low [1]-[10].

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The concentration and temperature dependence of the electron mobility in degenerate electron gas formed in Si(100) n-channel inversion layer has been experimentally obtained by Kawaguchi and Kawaji [11] for temperatures below 70 K and for the electron surface density $N_i > 10^{12}$ cm^{-2}. To interpret these experimental data, Shinba and Nakamura [12] have developed a comprehensive theory of phonon limited electron mobility in a degenerate 2DEG at low lattice temperature ($T_L < 50$ K). They have concluded that the surfon scattering mechanism alone cannot explain the experimental observations.

In semiconductor surface layer the Fermi energy ϵ_F of the free electrons is usually greater than their thermal energy and hence the electron system obeys the degenerate statistics. In a degenerate system the electrons with the corresponding Fermi energy are responsible to control the electrical transport characteristics in the system. 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 elastic in contrast to what is seen to be inelastic in a non-degenerate 2DEG system at lower temperatures [10]. 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],[13],[14].

A good number of theoretical investigations on the intravalley acoustic phonon scattering and the corresponding electrical transport characteristics in 2DEG systems have been made [4],[6],[9],[10],[15]. Lei *et al* [16] have developed a non-Boltzmann theory of the steady state transport using the full phonon distribution at low temperatures and obtained the transport characteristics in GaAs-$Ga_xAl_{1-x}As$ heterojunctions. However, in the study of electrical transport in 2DEG the true phonon population and the effect of screening due to free carriers are not taken into account with sufficient precision even at low lattice temperatures. In this article the theory of the intravalley acoustic phonon scattering of the electrons in a degenerate 2DEG system has been developed 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 theory has been applied to observe the temperature dependence of the electron mobility in a 2DEG formed in Si(100) n-channel inversion layer. The results thus obtained are compared with the available experimental [11] data and also with other theoretical [12] calculations.

II. THEORY

The conduction electrons in an 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 [6] as

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

where $\epsilon_{\vec{k}}$ is the energy of the electron, $\vec{k}$ is the component of the electron wave vector parallel to the interface. ħ 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 $E_s = eN_i/\epsilon_{sc}$, e being the electronic charge and ϵ_{sc} the permittivity of the semiconductor, $m_\perp^*$ is the effective mass perpendicular to the surface, and γ_n are the roots of the Airy function $A_i(-\gamma_n)$.

Usually at low temperatures with low carrier densities 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 conduction 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 phonon-limited momentum relaxation time $\tau_{ac}(\epsilon_{\vec{k}})$ of an electron with energy $\epsilon_{\vec{k}}$ in a degenerate 2DEG may be obtained from the perturbation theory as [6]

$$\frac{1}{\tau_{ac}(\epsilon_{\vec{k}})} = \frac{2\pi}{\hbar}\int_{\theta=0}^{2\pi}\int_{q_1}^{q_2} \frac{s}{(2\pi)^2}\Big[\left|\langle \vec{k}+\vec{q}|H'_{ac}|\vec{k}\rangle\right|^2 \times \{1 - f_0(\vec{k}+\vec{q})\}\delta(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} - \hbar q u_l) + \left|\langle \vec{k}-\vec{q}|H'_{ac}|\vec{k}\rangle\right|^2 \{1 - f_0(\vec{k}-\vec{q})\} \times \delta\big(\epsilon_{\vec{k}-\vec{q}} - \epsilon_{\vec{k}} + \hbar q u_l\big)\Big]\, q\, dq\, d\theta, \qquad (2)$$

where the squared matrix element of the electron-lattice scattering is given by

$$\left|\langle \vec{k}\pm\vec{q}|H'_{ac}|\vec{k}\rangle\right|^2 = \left(\frac{\mathcal{E}_a^2 \hbar q^2}{2 s d \rho_v \omega_q}\right) S^2(q)\left(N_q + \frac{1}{2} \pm \frac{1}{2}\right).$$

Here $\mathcal{E}_a$ is the effective deformation potential constant which assumes a value larger than that for the bulk material for higher-order subbands [6]. Vass *et al* [17] developed a theory to determine the surface deformation potential constant $\mathcal{E}_a$ in terms of a bulk value of the deformation potential $\mathcal{E}_1$ and concentration N_i as

$$\mathcal{E}_a = \mathcal{E}_1 + 2.5 \times 10^{-8} \times N_i^{2/3} \quad \text{eV}.$$

The parameter s is the surface area, d is the width of the layer of lattice atoms with which the electrons can interact, and ρ_v is the mass density. The frequency of the lattice vibration $\omega_q = u_l q$, $\vec{q}$ being the component of the phonon wave vector parallel to interface and u_l is the acoustic velocity. N_q is the phonon population. $f_0(\vec{k} \pm \vec{q})$ 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. q_1 and q_2 are respectively, the lower and upper limits of q. The function $S(q)$ is the screening factor 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],[13]

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

where for degenerate 2DEG

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

In a degenerate 2DEG, as mentioned earlier, the electrons with energy around the Fermi energy ϵ_F control the transport. The Fermi energy in degenerate 2DEG is usually seen to be much greater than the acoustic phonon energy. As an example, for inversion layer concentration of the order of 10^{12} cm^{-2} in Si(100) layer the Fermi energy ϵ_F is seen to be 6 meV which is almost two order higher than the acoustic phonon energy. Thus the electron-phonon collisions may be considered to be elastic in these systems and the phonon energy $\hbar\omega_q$ 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 easily be carried out yielding

$$\frac{1}{\tau_{ac}(\epsilon_{\vec{k}})} = \frac{\mathcal{E}_a^2 m_\parallel^*}{2\pi\hbar^2 d\rho_v u_l k}[1 - f_0(\vec{k})] \times \int_{q_1}^{q_2} \frac{(2N_q + 1)S^2(q) q\, dq}{[1 - (q/2k)^2]^{1/2}}. \qquad (3)$$

At low lattice temperatures the phonon distribution is given to a good approximation by the Laurent expansion of the form [18]

$$N_q(x) = \sum_{m=0}^{\infty} \frac{B_m}{m!} x^{m-1} \quad ; \quad x \le \bar{x}, \qquad \approx 0 \quad ; \quad x > \bar{x}, \qquad (4)$$

where $\bar{x} = \hbar q u_l / k_B T_L$, 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.(3) can be determined 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 are seen to be 0 and $2k$. Hence carrying out the integration one can obtain

$$\frac{1}{\tau_{ac}(\epsilon_{\vec{k}})} = \mathcal{A}_a \lambda [1 - f_0(\epsilon_{\vec{k}})] \mathcal{F}_m(\epsilon_{\vec{k}}). \qquad (5)$$

Here

$$\mathcal{A}_a = \left(\frac{\varepsilon_a^2 m_\parallel^{*3/2}}{4\sqrt{2}\hbar^3}\right)\left(\frac{1}{\pi d \rho_v u_l}\right)\left(\frac{k_B T_L}{\sqrt{\varepsilon_s}}\right)^2,$$

$$\varepsilon_s = \frac{1}{2} m_\parallel^* u_l^2, \quad \lambda = \frac{4\sqrt{\varepsilon_s}}{k_B T_L}.$$

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

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

$$= \sum_{m=0}^{\infty} \frac{2B_{2m}}{(2m)!} \left[\sum_{n=0}^{2m} (-x_s)^n \binom{2m+2}{n} \times \left\{J_{2m-n+1}\left(\frac{1}{x_s}\right) - J_{2m-n+1}\left(\frac{1}{x_s+\bar{x}}\right)\right\} + \sum_{n=2m+1}^{2m+2} (-x_s)^n \binom{2m+2}{n} \times \left\{I_{n-2m-1}\left(\frac{1}{x_s}\right) - I_{n-2m-1}\left(\frac{1}{x_s+\bar{x}}\right)\right\}\right]$$
$$+ \sum_{n=0}^{1} (-x_s)^n \binom{3}{n} \left\{J_{2-n}\left(\frac{1}{x_s+\bar{x}}\right) - J_{2-n}\left(\frac{1}{x_s+x_c}\right)\right\} + \sum_{n=2}^{3} (-x_s)^n \binom{3}{n} \left\{I_{n-2}\left(\frac{1}{x_s+\bar{x}}\right) - I_{n-2}\left(\frac{1}{x_s+x_c}\right)\right\}; \quad \text{for } x_c > \bar{x}. \qquad (6)$$

Here

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

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

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

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

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

$$\Delta = 4ac - b^2, \quad R(x) = a + bx + cx^2,$$
$$a = -1, \quad b = 2x_s, \quad c = x_c^2 - x_s^2,$$
$$\binom{m}{n} = \frac{m(m-1)\ldots.(m-n+1)}{n!}, \quad \binom{m}{0} = 1.$$

When the screening effect is neglected one should put $S(q) = 1$ in Eq.(3) and then $\mathcal{F}_m(\epsilon_{\vec{k}})$ can be given as

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

$$= \sum_{m=0}^{\infty} \frac{2B_{2m}}{(2m)!} \mathcal{C}_{2m}(\bar{\theta}) x_c^{2m} + x_c \cos\bar{\theta}; \quad \text{for } x_c > \bar{x}. \qquad (7)$$

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

$$\mathcal{F}_m(\epsilon_{\vec{k}}) = 2\left[J_1\left(\frac{1}{x_s}\right) - J_1\left(\frac{1}{x_s+x_c}\right)\right] - 4x_s\left[I_0\left(\frac{1}{x_s}\right) - I_0\left(\frac{1}{x_s+x_c}\right)\right] + 2x_s^2\left[I_1\left(\frac{1}{x_s}\right) - I_1\left(\frac{1}{x_s+x_c}\right)\right], \qquad (8)$$

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

$$\mathcal{F}_m(\epsilon_{\vec{k}}) = \pi. \qquad (9)$$

If the electron distribution becomes degenerate the phonon-limited electron mobility in the surface inversion layer is given by [12]

$$\mu_{ac} = \frac{e\tau_{ac}(\epsilon_F)}{m_\mu^*}, \qquad (10)$$

with the Fermi energy $\epsilon_F = \pi\hbar^2 N_i / n_v m_\parallel^*$, n_v is the number of equivalent valleys at the surface.

III. RESULT AND DISCUSSION

For an application of the above theory, an n-channel (100) oriented Si inversion layer is considered with the material parameter values [10] : $\mathcal{E}_1 = 9$ eV, $u_l = 9.037 \times 10^3$ m s^{-1}, $\rho_v = 2.329 \times 10^3$ kg m^{-3}, $\epsilon_{sc} = 11.9$, longitudinal effective mass $m_l^* = 0.96 m_0$, transverse effective mass $m_t^* = 0.19 m_0$, m_0 being the free electron mass. At low lattice temperatures one may consider presumably the electrons occupy only the lowest subband when the layer thickness d is given by $(\hbar^2\epsilon_{sc}/2m_\perp^* e^2 N_i)^{1/3}\gamma_0$. For the (100) surface of Si the six valleys are not equivalent. The two equivalent valleys for which $m_{\parallel}^* = m_t^*$, $m_{\perp}^* = m_l^*$ and $m_{\mu}^* = m_t^*$ occupy the lowest subband [1],[3],[6].

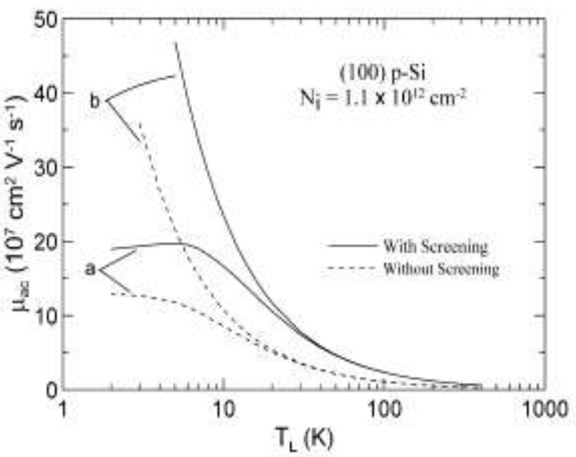

Fig.1 : Lattice temperature dependence of intravalley acoustic phonon limited zero-field electron mobility in (100) Si inversion layer. Letters a and b indicate respectively the contribution from the full phonon spectrum and its equipartition approximation.

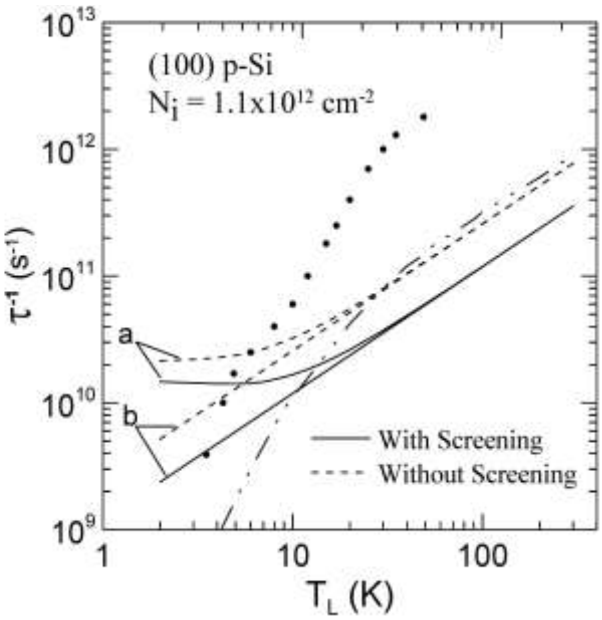

Fig.2 : Lattice temperature dependence of intravalley acoustic phonon scattering rate of free electrons with Fermi energy in (100) Si inversion layer. Symbols are from Experiment [11], dash-dot curve is from the theory of Shinba and Nakamura [12]. Letters a and b indicate respectively the contribution from the full phonon spectrum and its equipartition approximation.

The effect of screening of the free electrons on the electron mobility in a 2DEG controlled by the acoustic phonons at different temperatures is plotted in Fig.1. From the figure it is observed that the mobility values obtained giving due account to the screening effect are significantly greater whether the equipartition approximation of the phonon distribution is considered or not. Again as expected, the screening effect is more significant lower the lattice temperature. It is also noted that the qualitative change in the shape of the mobility characteristics is absent whether the equipartition law is taken under consideration or not, but at lower temperatures the mobility values obtained under the equipartition law decrease sharply in comparison to those obtained when the full phonon spectrum is taken into account.

In Fig.2 the temperature dependence of the scattering rate of free electrons with Fermi energy ϵ_F obtained from the present theory has been compared with the experimental [11] and theoretical results [12] above 2K. It may be noted that the theory developed here considering the bulk phonons which do not interact dominantly with free electrons at very low lattice temperatures. However, at very low lattice temperatures the Rayleigh wave phonons play significant role in controlling the electron transport in surface layers [12].

IV. CONCLUSION

From Fig.2 it is obvious that none of the theoretical results agrees with experimental data. The reason behind the disagreement has been elucidated by Shinba and Nakamura [12] pointing out the fact that at low temperatures, the electron mobility in 2DEG cannot be attributed to the surface phonon scattering only. This apart, the independent studies on the information about the phonon parameters in the surface region are necessary to properly explain the electron transport in 2DEG.

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