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Mobility of electrons in a quantized silicon inversion layer due to phonon scattering

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A theory for the mobility limited by lattice scattering in a quantized silicon inversion layer is developed in this paper. The expression for the relaxation time for scattering of a degenerate two-dimensional electron gas by a nonpolar optic phonon is derived from the Boltzmann equation and is found to differ from those given by other workers. The wave vectors of different phonons participating in the intersubband and intervalley transitions in a (100)-oriented silicon surface are then estimated by following a geometrical construction and considering the lowest three subbands. The dispersion curves for bulk phonons are used to determine the phonon temperatures. By taking an acoustic phonon and an averaged low-energy and an averaged high-energy phonon, the mobility is calculated by using both the nondegenerate and degenerate statistics. It is found that the mobility values are different for the two cases even at 300 K.

I. INTRODUCTION

Under the influence of a strong gate bias, the electrons in the inversion layer of a metal-oxide–semiconductor field-effect transistor (MOSFET) behave as a two-dimensional electron gas (2DEG). The electronic motion perpendicular to the surface gets quantized in discrete energy levels and remains free, parallel to the surface. In recent years, study of the electronic properties of this 2DEG[1] has received a good deal of attention from many workers. MOSFET structures employing different semiconductors have been used; however, among all, silicon is the most widely studied material.

Transport in the 2DEG formed in the silicon inversion layer has been studied by many workers[2-10] for different values of gate voltage, temperature, and substrate bias. A large number of theoretical papers[4-7,10-18] have appeared in the literature pointing out the importance of different scattering mechanisms. It is the general conclusion that phonon scattering in conjunction with scattering due to surface roughness and by surface-oxide charges may be considered to calculate the mobility and other transport coefficients of the 2DEG. In earlier works, it was assumed that scattering via the deformation-potential acoustic phonon is the only lattice-scattering mechanism. However, the importance of intersubband and intervalley scattering which involve energetic phonons was realized soon and given due consideration by different workers.[10,12,17,18] Sah *et al.*[10] considered the transport in a weakly inverted surface and extracted the values of the lattice-scattering-limited mobility, μ_L, from their experimental data μ_{expt}, and calculated mobility due to surface-oxide-charge scattering, μ_I, by employing Matthiessen's rule. They then derived an expression for the relaxation time due to optic-phonon scattering for a nondegenerate electron gas. Considering a single optic phonon of temperature 650 K, they obtained the value of the coupling constant for the optic phonon from their extracted value of mobility. The work of Sah *et al.* cannot, however, be applied to the most general case, because a single optic phonon cannot represent all the intersubband and intervalley transitions, and moreover, the expressions are valid for a nondegenerate electron gas. It should also be noted that the assumption of Matthiessen's rule leads to an incorrect value of the coupling constant.[19] Ezawa *et al.*[12] made a rough estimate of mobility by using phonon temperature and coupling constants that were used in calculating the transport parameters in bulk Si.

Recently Ferry[17,18] made a detailed calculation of mobility by assuming that the same g and f scattering[20] which occur in bulk silicon are responsible for the intersubband and intervalley transitions in the quantized layers. He then derived expressions for the relaxation time appropriate for a 2DEG obeying Fermi statistics. By employing the bulk values of the coupling constants for g-type and f-type phonons, Ferry[17] computed the values of mobility in the nondegenerate approximation and claimed good agreement with the lattice-scattering-limited mobility extracted by Sah *et al.*[10]

In the quantized inversion layers, the electron motion is two-dimensional in nature and the disposition of valleys in the two-dimensional Brillouin zone is quite different from that in the bulk.[21] The wave vectors and energies of different phonons causing intersubband and intervalley transitions are, therefore, likely to be different from those in the bulk. The model employed by Ferry for the two-dimensional inversion layer therefore needs further examination. Also, the expression given by him for the relax-

ation time due to energetic phonon scattering for degenerate statistics is incorrect.[22,23] Ferry assumed nondegenerate statistics in the final computation. However, most of the electrons in the lowest subband E_0 for (100) Si surface are below Fermi level. The computed values of mobility are likely to be different if degenerate statistics are considered. It is also to be noted[19] that the values of mobility obtained by Sah *et al.* cannot be accepted as the correct values of lattice-scattering-limited mobility. Therefore the agreement claimed by Ferry between his calculated results and the results of Sah *et al.* is not of much significance.

The foregoing discussion points out that a proper theory of transport due to lattice scattering in the silicon inversion layer is still lacking. The correct expression for the relaxation time of a degenerate 2DEG due to scattering by energetic phonons is not available in the literature. Also, the phonons which are responsible for intersubband and intervalley transitions in the 2DEG have not been identified. The purpose of the present paper is to investigate along this line and present the results. Section II gives the derivation of relaxation time due to scattering by energetic phonons by considering the degeneracy of 2DEG. In Sec. III, the procedure for obtaining the wave vectors and temperatures of the phonons, relevant for conduction in the (100)-oriented silicon surface, is discussed. An estimate of the difference in mobility values calculated with degenerate and nondegenerate statistics is given in Sec. IV. Finally, the conclusions of the present study are presented in Sec. V.

II. RELAXATION TIME FOR OPTICAL-PHONON SCATTERING IN A DEGENERATE 2DEG

The rate of change of the distribution function $f(\vec{k})$ due to collision may be written as[24]

$$\left.\frac{\partial f(\vec{k})}{\partial t}\right|_{\text{Coll}} = -\frac{A}{(2\pi)^2}\int \{P(\vec{k},\vec{k}')f(\vec{k})[1-f(\vec{k}')] - P(\vec{k}',\vec{k})f(\vec{k}')[1-f(\vec{k})]\}d\vec{k}', \tag{1}$$

where A is the area of the surface, $\vec{k}$ is the two-dimensional wave vector of the electrons, and $P(\vec{k},\vec{k}')$ and $P(\vec{k}',\vec{k})$ are the probability per unit time of transfer from $\vec{k}$ to $\vec{k}'$ and from $\vec{k}'$ to $\vec{k}$, respectively. We assume that the distribution function may be expanded as

$$f(\vec{k}) = f_0(E) + kf_1(E)\cos\theta\,, \tag{2}$$

and

$$f(\vec{k}') = f_0(E) + k'f_1(E')\cos\theta'\,, \tag{3}$$

where E is the energy and θ and θ' are the angles made by $\vec{k}$ and $\vec{k}'$, respectively, with the electric field. Substituting Eqs. (2) and (3) in (1), using the principle of detailed balance, and neglecting the products $f_1(E)f_1(E')$, we can write Eq. (1) as

$$\left.\frac{\partial f(\vec{k})}{\partial t}\right|_{\text{Coll}} = -\frac{A}{(2\pi)^2}\int \left(P(\vec{k},\vec{k}')\frac{1-f_0(E')}{1-f_0(E)}f_1(E)k\cos\theta - P(\vec{k},\vec{k}')\frac{f_0(E)f_1(E')}{f_0(E')}k'\cos\theta'\right) \times d\vec{k}'. \tag{4}$$

For two dimensions $d\vec{k}' = k'dk'd\beta$ and

$$k'\cos\theta' = k'\cos\beta\cos\theta + k'\sin\beta\sin\theta\,,$$

where β is the angle between $\vec{k}$ and $\vec{k}'$ which varies from 0 to 2π.

The matrix element for transition from $\vec{k}$ to $\vec{k}'$ involving an optical phonon is given by[17]

$$|\langle\vec{k}'|H|\vec{k}\rangle|^2 = (D_R^2\hbar I/2A\rho\omega_R d) \times (N_R + \tfrac{1}{2} \mp \tfrac{1}{2})\delta(E_{\vec{k}} - E_{\vec{k}'} \mp \hbar\omega_R)\,, \tag{5}$$

where D_R is the deformation potential constant, ω_R is the frequency of the relevant phonon mode, N_R is the phonon occupation number, ρ is the density, d is the average thickness of the inversion layer, and I is the overlap integral. The positive and negative signs in Eq. (5) correspond, respectively, to the emission and absorption processes. The matrix element given by Eq. (5) is appropriate for a randomizing collision. Thus Eq. (4) when integrated over β reduces to

$$\left.\frac{\partial f(\vec{k})}{\partial t}\right|_{\text{Coll}} = -\frac{Akf_1(E)\cos\theta}{2\pi}\int P(\vec{k},\vec{k}')\frac{1-f_0(E')}{1-f_0(E)}k'dk'. \tag{6}$$

For a randomizing collision a relaxation time τ can be defined and Eq. (6) reduces to

$$\left.\frac{\partial f(\vec{k})}{\partial t}\right|_{\text{Coll}} = -\frac{k\cos\theta f_1(E)}{\tau}\,, \tag{7}$$

where

$$\frac{1}{\tau} = \frac{A}{2\pi}\int P(\vec{k},\vec{k}')\frac{1-f_0(E')}{1-f_0(E)}k'dk'. \tag{8}$$

From the E-$\vec{k}$ relation of 2DEG one may write

$$k'dk' = (m_D'/\hbar^2)dE'\,, \tag{9}$$

where m_D' is the density-of-states effective mass of the electrons. Using Eqs. (5), (8), and (9) and integrating over energy space we get

$$\frac{1}{\tau}=\frac{D_R^2 m_D' I}{2\rho\hbar^2 d}\left((N_R+1)\frac{1-f_0(E-\hbar\omega_R)}{1-f_0(E)}u(E-\hbar\omega_R-E_i)+N_R\frac{1-f_0(E+\hbar\omega_R)}{1-f_0(E)}u(E+\hbar\omega_R-E_i)\right), \tag{10}$$

where u is a step function $[u(<0)=0,\ u(>0)=1]$. Equation (10) is the correct expression[22] for the relaxation time of a degenerate 2DEG due to optical-phonon scattering. It differs from the expressions derived by other workers simply by including a factor $[1-f_0(E')]$ in the corresponding expressions for a nondegenerate gas.

III. INTERSUBBAND AND INTERVALLEY SCATTERING IN A (100)-ORIENTED SILICON SURFACE

Assuming that the surface potential varies linearly with distance from the oxide-silicon interface (the triangular potential approximation), the energy of the quantized electronic subband is given by[21,25]

$$E_i=(\hbar^2/2m_z^*)^{1/3}[\tfrac{3}{2}\pi eF_s(i+\tfrac{3}{4})]^{2/3},\quad i=0,1,2,\ldots \tag{11}$$

where F_s is the surface electric field and m_z^* is the effective mass along the z direction, the direction perpendicular to the interface. For a multivalley semiconductor like Si, having a (100)-oriented surface, two out of six degenerate valleys have their longitudinal mass $m_l=m_z^*$ (type I valleys). The lowest subband E_0 and the next higher subband E_1 are due to these two valleys. The remaining four valleys (type II valleys) having their transverse mass $m_t=m_z^*$ give rise to the next higher subband $E_{0'}$. $E_{0'}$ contains four degenerate valleys having ellipsoidal constant-energy contours. The energies of E_1 and $E_{0'}$ are very close to each other[25] for a wide range of temperature and carrier concentration and we shall assume that these two subbands have identical energies. We shall consider the above three subbands only. The dispersion relation in the subband $E_{0'}$ is

$$E(\vec{k})=E_i+\frac{\hbar^2k_x^2}{2m_x^*}+\frac{\hbar^2k_y^2}{2m_y^*}. \tag{12}$$

For E_0 and E_1 the above relation holds true with $m_x^*=m_y^*=m_t$.

Figure 1 gives a schematic representation of different constant-energy contours and Brillouin zone for the (100) surface of silicon.[21] Figure 1(a) depicts the lowest E_0 subband with two degenerate valleys at the zone center. Figure 1(b) is for the combination of E_1 and $E_{0'}$ subbands and depicts two degenerate valleys at the zone center and four degenerate valleys along the [100] and [010] directions with their extrema at $0.85k_{max}$ (Ref. 26) away from the center.

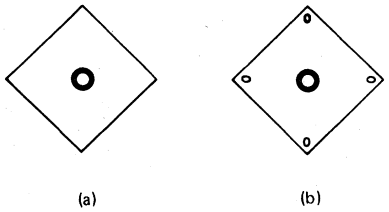

FIG. 1. Schematic representation of the constant-energy contours and Brillouin zones for the (100) surface of Si: (a) constant-energy circles for E_0 layer, (b) constant-energy contours for E_1 and $E_{0'}$ layers, assumed to have the same energy. The radii of the circumscribed circles about the Brillouin zones are $2\pi/a$.

The possible inter- and intrasubband scattering processes may now be described with the aid of Fig. 2. The phonon wave vectors may be determined by following a geometrical construction. A similar method[20] was employed earlier for bulk Si for the same purpose. The transition designated by V is a vertical one which may or may not involve the zone-center optical phonon. The phonon wave vector responsible for the process A is obviously $0.85q_{max}$ along the [100] direction. Figure 2(b) indicates the transitions occurring in the E_1 subband. Process B is identical with process A. It may easily be verified that transitions designated as C and D are umklapp processes. The transition from valley 3 to valley 1 may be viewed as the transition from valley 3 to valley 1′ in the adjacent zone and then from 1′ to 1 by the absorption of a principal lattice vector. The wave vector responsible for transition from 3 to 1 is $0.3q_{max}$ along the [100] direction. Similarly, transition from valley 3 to valley 2 may be thought of

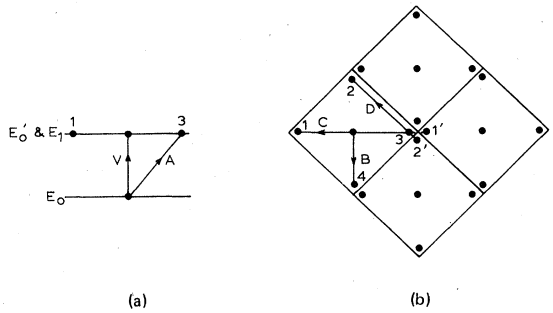

FIG. 2. Possible inter- and intrasubband transitions. (a) indicates transitions from E_0 layer to the combination of E_1 and $E_{0'}$ layers. (b) Depicts the intrasubband transitions in the E_1 and $E_{0'}$ layers. The positions of the extrema are indicated by solid circles. 13 and 24 are along the [100] and [010] directions, respectively.

as a transition from valley 3 to valley 2′ in the adjacent zone with the aid of a phonon of wave vector $\sqrt{2} \times 0.15(2\pi/a)$ along the [110] direction, transition from valley 2′ to valley 2 being a virtual process. The temperatures of the phonons participating in all the processes described above may be found out from the dispersion curves. It is expected that the electrons would be scattered by the phonons excited near the surface, the dispersion relation for which may be different from that of bulk phonons. In the absence of any data on surface phonons, we use the dispersion curves for bulk phonons.[27,28] Table I includes the wave vectors and temperatures of all the phonons involved in the above processes. Some of the phonons may, however, be excluded in the actual case, if proper selection rules are taken into consideration. The selection rules in the present case are not known and we shall consider some kind of average of all the phonons listed in Table I for our calculation.

IV. DISCUSSIONS

The results given in Secs. II and III cannot be used immediately for calculation of mobility, since the values of deformation potential constant D_R appearing in Eq. (10) for all the phonons listed in Table I are not known. These constants are to be obtained from the experimental values of mobility which is limited by, in addition to lattice scattering, surface-roughness and surface-oxide-charge scattering. The usual procedure is to treat D_R's as adjustable parameters and calculate and compare the values of mobility, obtained by considering all the scattering processes with the experimental values. The theory of roughness[29] and oxide-charge scattering[21] is reported in the literature. The relaxation time for roughness scattering, however, contains adjustable parameters. To reproduce the mobility-temperature and mobility-gate voltage data by a proper choice of all the adjustable parameters is quite a tedious and time-consuming job and we do not make any such attempt in this paper. Instead, we investigate in the present work how the mobility values differ when the two statistics are considered.

We consider that the electrons in the three subbands are scattered by deformation-potential acoustic and intervalley phonons. We neglect the contributions due to intravalley optical (zone-center) phonon scattering as well as those due to transition from E_0 to E_1 subband via a zone-center optic phonon (process V in Table I). We are assuming the wave function to be Airy-function-type, for which the overlap integral for transition from E_0 to E_1 vanishes,[17] and therefore V processes do not make any overall contribution. We also assume that a 215-K phonon and a 620-K phonon account for the transition from the E_0 to $E_{0'}$ (also from E_1 to $E_{0'}$) subband. Transition from one valley in $E_{0'}$ to the opposite one involves a 150-K phonon, while from the same valley to each of the two perpendicular valleys it is accomplished with the aid of a 720-K phonon. The phonons are a kind of average of the phonons listed in Table I.

Using the expression for relaxation time for acoustic-phonon scattering given by Kawaji[11] and Eq. (10), we can calculate $\langle\tau\rangle$, the averaged relaxation time, as

$$\langle\tau\rangle_j = \int_{E_j}^{\infty} E\tau \frac{\partial f_0}{\partial E}\, dE \Big/ \int_{E_j}^{\infty} f_0(E)dE . \tag{13}$$

The overall mobility becomes

$$\mu_{\text{eff}} = \frac{e}{N_{\text{inv}}} \sum n_j \langle\tau\rangle_j / m_{cj}, \quad j = 0, 1, 0' .$$

m_c is the conductivity effective mass, and the total inversion layer concentration N_{inv} is given by

TABLE I. Wave vector and temperature of the phonons involved in intra- and intersubband scattering in (100)-oriented silicon surface.

Process	Transition	Wave vector	Direction	Phonon temperatures (K) for modes TA	LA	LO	TO
V	E_0 to $E_{0'}$	0				740	740
A	E_0 to $E_{0'}$	0.85 $(2\pi/a)$	[100]	215	525	620	680
B	E_1 to $E_{0'}$	0.85 $(2\pi/a)$	[100]	215	525	620	680
C	Between opposite valleys in $E_{0'}$	0.3 $(2\pi/a)$	[100]	135	225	720	720
D	Between perpendicular valleys in $E_{0'}$	$\sqrt{2} \times 0.15$ $(2\pi/a)$	[110]	110	175	725	725

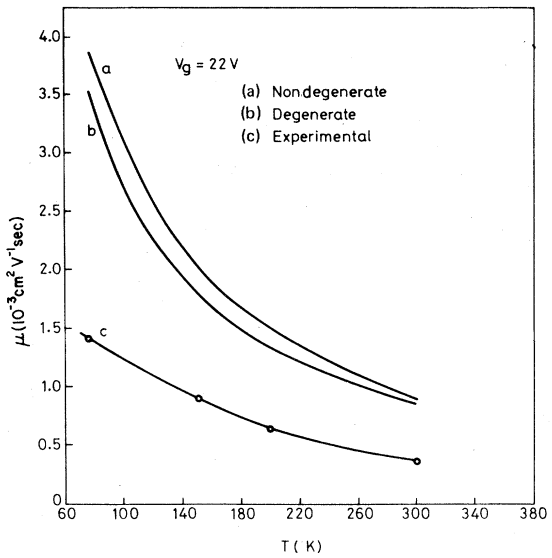

FIG. 3. Effective mobility versus temperature in the (100)-oriented silicon inversion layer for an effective gate voltage assuming (a) nondegenerate, (b) degenerate statistics, and compared with experimental results (c).

$$N_{\text{inv}} = \frac{g_s g_v k_B T}{2\pi\hbar^2} \sum_i m_{D_i} \ln\left[1 + \exp\left(\frac{E_f - E_i}{k_B T}\right)\right] . \tag{14}$$

g_s and g_v are, respectively, the spin and valley degeneracy factor. The effective mobility has been calculated for (100)-oriented silicon layer by using the following values of parameters: $m_t = 0.190 m_0$, $m_l = 0.916 m_0$, $g_s = 2$, $g_v = 2$ for E_0 and E_1 subbands and $g_v = 4$ for the E_0' subband, $\rho = 2.33$ g/cm^3, $u_l = 8.476 \times 10^5$ cm/sec, $N_{\text{inv}} = 10^{12}$ cm^{-2}. D_R for 150-K and 215-K phonons is equal to 0.8×10^8 eV/cm; D_R for 620-K and 720-K phonons is equal to 9×10^8 eV/cm.[30]

The calculated values of mobility are shown in Fig. 3. It is seen that the values with degenerate statistics differ from those with nondegenerate statistics. In the present case, only the E_0 subband is below E_F, and mobility for this subband only is changed due to different forms of $f_0(E)$. The difference exists even at 300 K. It is to be noted that the difference of mobility values displayed in Fig. 3 will vary in magnitude if D_R values different from those given above are used.

V. CONCLUSIONS

We have presented a correct expression for the relaxation time of a degenerate 2DEG due to nonpolar-optic-phonon scattering and obtained the values of phonon temperatures for intersubband and intervalley transition in (100)-oriented Si surface. Values of mobility calculated with Fermi statistics are found to differ from those calculated with Boltzmann statistics.

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