CHANNEL MOBILITY IN SILICON MOSFETs

C Moglestue

GEC Research Limited, Hirst Research Centre, Wembley, Middlesex HA9 7PP, United Kingdom

ABSTRACT

The theory of mobility of electrons and holes in inversion layers formed at the interface between a semiconductor and an insulator has been reviewed in terms of interaction of the current with surfons and ionised impurities. The carriers move in a quantum well defined by the interface potential. The shape of this well has been calculated by the simultaneous solution of Poisson's and Schrödinger's equations under the assumption that the population of the subbands obey Fermi-Dirac statistics. It has been necessary to assume that the surface deformation potential is different from that in the bulk; this is reasonable as both the deformation of the crystal structure at the interface and the surfons contribute to it.

The variation of the low longitudinal field mobility with both perpendicular electric field and temperature has been compared with measurements. For the former the agreement is good except at the low fields present close to threshold bias. The temperature dependence for the electrons also agrees well with experimental data, but the calculated mobility for the holes is less sensitive to temperature variations than that measured. The ionised impurity scattering does not contribute significantly to the mobility at room temperature for doping densities below 10^{22} m^{-3}.

1 INTRODUCTION

During the last twenty years attention has been paid to the quantum mechanical calculation of the distribution of the conduction electrons at the interface between the semiconducting silicon and the insulating oxide [1,2]. When the gate bias is sufficiently strong that the edge of the

conduction band of the p-type semiconductor is bent below the Fermi level, the electron current can flow. The band structure has been reviewed by Ando [3]. When current flows, the electric field perpendicular to the interface is sufficiently strong that a quantum well forms, in which the conduction band splits into subbands, Figure 1. Quantum theory predicts that the electron density will peak a few atomic distances from the interface, in contrast to the classical picture with the highest electron density at the interface itself. At low temperatures, this quantisation has been seen experimentally [4], and also at room temperature [5].

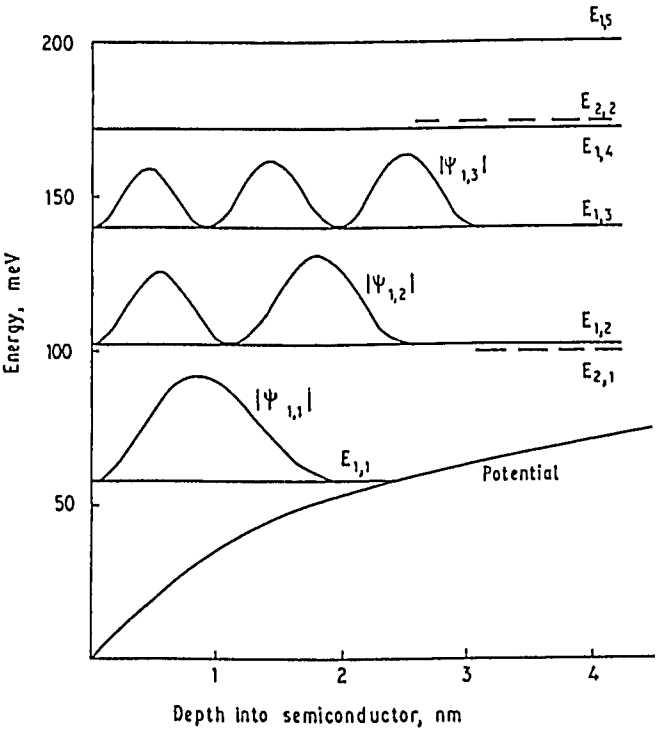

Figure 1: The shape of the potential well at a uniform doping density at 10^{20} m^{-3} and perpendicular interface electric field of 20 MVm^{-1}. The horizontal lines represent the energy levels and the shape of the electron distribution has been drawn for the three lowest rungs of the light electron ladder. The Fermi level is at +2 meV.

For holes, such a study has not been carried out. The hole current at the surface of an n-type semiconductor is established by biasing the gate sufficiently negative to cause the top of the valence band to lift above the Fermi level.

Ezawa et al [6] have introduced a theory describing the mobility versus the perpendicular electric field which has met with limited success; the predicted mobility is higher than the observed one. Shinba et al [7] suggested that an additional scattering mechanism has to be included, but have not investigated it in detail.

The purpose of this paper is to re-examine the quantum mechanical mobility theory for both electrons and holes in the effective mass approximation, considering interaction with phonons and ionised impurities, and the occupancy of all subbands. The confinement of carriers within well separated subbands ensures that the scattering is two dimensional; a surface rather than bulk scattering rate must then have to be used.

The band structure from the self consistent solution of Schrödinger's and Poisson's equations will be presented in the next section. The rates of scattering from all processes considered will be discussed in Section 3. The mobilities for holes and electrons versus the perpendicular electric field and for zero longitudinal field will be calculated in Section 4 and compared with experimental values in Section 5. The last two sections will contain a discussion of this comparison and a conclusion.

2 THE BAND STRUCTURE

Consider a p-type silicon semiconductor with a planar surface of sufficiently large extent to be able to neglect effects of the edges. This is covered by an insulating oxide of uniform thickness, which in turn is covered by positively biased metal. This bias causes the conduction and valence bands of the semiconductor to be bent; when the bias is sufficiently large, the conduction band edge bends below the Fermi level, Figure 1, so that an electron current can flow. (In an n-type semiconductor a hole current can be made to flow by biasing the metal sufficiently negative to bend the valence band above the Fermi level.) If the sheet charge density of depleted holes is N_{depl} and the charge density of conduction electrons is N_{inv} then the electric field at the interface is

$$F_s = e(N_{inv} + N_{depl})/(\varepsilon\varepsilon_o) \qquad (1)$$

Where $\varepsilon\varepsilon_o$ is the dielectric permittivity of the semiconductor and e the elementary electronic charge. Above threshold, N_{depl} stays constant, while N_{inv} varies with the bias. A quantum well forms near the interface between the semiconductor and the insulating oxide, in which the conduction band splits up into subbands.

The charge distribution defines the potential, ϕ, in the semiconductor through the one dimensional Poisson's equation

$$\frac{d^2\phi}{dz^2} = \frac{-\rho(z)}{\varepsilon\varepsilon_o} \tag{2}$$

where z is reckoned positive into the semiconductor and $\rho(z)$ is the charge distribution, which is determined from the Schrödinger equation remaining when the transversal components have been eliminated [2]:

$$\frac{d^2\psi_{ik}}{dz^2} = \frac{2m^*}{\hbar^2}\,[E_{ik}-e\phi(z)]\psi_{ik} \tag{3}$$

Here m^* represents the effective mass of the electron and E_{ik} the eigenvalue corresponding to the eigenfunction ψ_{ik}, in other words; E_{ik} is the energy of the bottom of level k in ladder i. For (100) oriented silicon, ladder 1 consists of the levels from the (100) ellipsoids and ladder 2 of those from the (010) and (001) ones. In this orientation an electron of wave vector $\underline{k}$ relative to the centre of the ellipsoid has energy

$$E'_{ik} = E_{ik} + \tfrac{1}{2}\hbar^2\,(k_x^2/m^*_{ix} + k_y^2/m^*_{iy}) \tag{4}$$

where k_x and k_y represent perpendicular components of $\underline{k}$ parallel to the interface and m^*_{ix} and m^*_{iy} the effective masses in these directions in subband ladder i

The charge entering Eq (2) is given by

$$\rho(z) = e\int_{-\infty}^{\infty} dz\,\Big[\sum_{ik} n_{ij}\,|\psi_{ik}(z)|^2 + \rho_{dop}(z)\Big] \tag{5}$$

where ρ stands for the depletion density of the semiconductor, which is taken to be uniform and equal to the doping density down to a constant depth, and then zero. The occupation of level k of ladder i is

$$n_{ik} = \int_{E_{ik}}^{\infty} dE\; f(E)D(E) \tag{6}$$

where

$$f(E) = \{1+\exp[(E-E_F)/(k_BT)]\}^{-1} \tag{7}$$

which applies when the electric field parallel to the interface is sufficiently weak. The density of states is

$$D(E) = 2g\sqrt{m_x m_y}/(2\pi\hbar^2) \qquad (8)$$

where E_f represents the Fermi energy, k_B Boltzmann's constant and T the temperature. The factor 2g allows for the surface degeneracy.

Equations (2) and (3) have been solved previously [8], subject to the conditions (1), (5-8), $\phi(0)=0$ and $\psi_{ij}(-\infty)=\psi_{ij}(\infty)=0$. Figure 1 also shows the charge distribution $|\psi_{ij}(z)|^2$ for the lowest subbands, together with the energy levels in the quantum well. $|\psi_{ij}(z)|^2$ expresses the probability of finding an individual particle at depth z from the interface, this probability peaks some nanometres into the semiconductor. The perpendicular component of momentum is undefined. When the temperature is sufficiently low that only the few lowest subbands are populated, the transport can be considered two dimensional.

3 TRANSPORT

As the electrons are restricted thus, they cannot receive any momentum out of their plane. Any interacting phonon therefore also has to propagate parallel to the surface. Such bulk phonons are highly improbable, but as phonons reach the surface, they split; one part is reflected into the material and the other continues along the interface [9].

Using the Golden rule, the matrix element found from the deformable-ion model yields, along lines followed by Ezawa et al [10] and Ferry [11], the rate of quasi-elastic surfon scattering within level k of ladder i which is of width w_{ik}:

$$\lambda_a = \frac{\Xi^2 K_B T m_i^*}{\hbar^3 w_{ik} \rho u^2} \exp(-2\alpha k w_{ik}) \qquad (9)$$

where Ξ represents the surfon deformation potential, which is not the same as the bulk one, as the lattice at the interface is distorted through the crystallographic mismatch between semiconductor and the oxide. The quality of this interface depends on the way it was formed. The density of the crystal is represented by ρ, and u is the surfon velocity. The surfon amplitude attenuation factor α expresses the penetration of the lattice distortion created by the surfon into the bulk, this distortion is felt by the electron.

The phonons in the oxide also split into a surfon and a reflected or refracted phonon. This surfon also interacts

with inversion carriers at a rate given by an expression similar to Eq (9), so that this equation thus represents the combined effects of semiconductor and oxide surfons. Electrons can also be transferred from subband (i,k) to (j,l) by means of surfons originating from f and g phonons in the silicon. The rate of this transfer is:

$$\lambda_{ki} = \frac{\Xi_p^2 m_j^* I_{ij}^{kl}}{\hbar^2 \omega \rho w_{ik}} \exp(-2\alpha k w_{ik}) \; (N_{ik}+\tfrac{1}{2}\pm\tfrac{1}{2}) \; \theta \; (E_{ik}-E_{jl}\pm\hbar\omega) \quad (10)$$

where

$$I_{ij}^{kl} = \left[\int dz \; \psi_{ik}^*(z) \; \psi_{jl}(z)\right]^2 \quad (11)$$

represents the overlap between ψ_{ik} and ψ_{jl}. As the wavefunctions ψ_{ik} are orthogonal within the same energy ladder, $I_{ij}^{kl}=\delta_{kl}$, so that scattering between subbands within a ladder cannot take place, in contrast with Terashima and Hamaguchi [12], who wrongly take $I_{ij}^{kl}=1$ for all transitions. The transfer has to take place by transition between different ladders.

The phonon occupation number N_{ik} is given by the Bose-Einstein statistical distribution

$$N_{ik} = \{\exp[\hbar\omega/(K_B T)]-1\}^{-1} \quad (12)$$

The positive and negative components of the double sign correspond to surfon creation and annihilation, respectively, and the step function $\Theta(x)=1$ for $x>0$, 0 otherwise. The energy E of the carrier is reckoned from the bottom of the energy band in which it resides prior to scattering. Ξ_p represents the f or g phonon deformation potential.

The crystalline symmetry prohibits electrons from interacting with the optical phonons in the semiconductor. However, the optical phonons in the oxide are polar, the effect of the polarisation they create is felt by the electron current. Their rate of interaction is [13]:

$$\lambda_{rip} = \frac{m_i^* e^2 \omega_o}{4\pi\varepsilon_o \hbar^2} \exp(-2\alpha k w_{ik}) \left(\frac{1}{\varepsilon_\infty+\varepsilon} - \frac{1}{\varepsilon_x+\varepsilon}\right) \int_0^{2\pi} d\theta \left(\frac{b}{b+q_o}\right)^6 \frac{1}{q_o}$$

$$\theta \; (E_{jl}\pm\hbar\omega_o)(N_{ij}+\tfrac{1}{2}\pm\tfrac{1}{2}) \quad (13)$$

with q_o and ω_o representing the magnitude of the wave vector and the angular frequency of the optical oxide phonon, respectively, ε_∞ and ε_x the high and low frequency dielectric constants, respectively, of the oxide and $b = 3/w_{ik}$. N_{ik} is given by Eq (12).

Assuming the Brooks-Herring screened potential from ionised impurities, the rate of the elastic scattering from the impurities in the channel is:

$$\lambda_{ii} = \frac{m^* w_{ik} n}{\hbar^3(\beta^2+k^2)} \quad \frac{e^2}{\varepsilon\varepsilon_o} \tag{14}$$

where β is the screening length, n the bulk doping density, and k the magnitude of the carrier wave vector. Ionised impurities in the oxide and trapped charges also cause scattering, but their rate is sufficiently low to be neglected. This also applies to carrier-carrier scattering and scattering from crystalline defects and neutral impurities. Roughness scattering will not be included as an evaluation of its rate is not much better than a guess. Any effect of irregularities at the interface will be attenuated as the carriers move at a distance from it. With today's technology it is possible to manufacture sufficiently smooth interfaces that the contribution from roughness scattering can be made insignificant.

For holes the constant energy surfaces stay near the centre of the Brillouin zone. All transfers within and between subbands are caused by acoustic surfons originating from phonons in both sides of the interface. The quasi elastic intraband transitions have a rate given by Eq. (9), and the rate of interband scattering is:

$$\lambda_{ki} = 2\,\frac{\Xi_h^2 K_B T m_j^*}{\hbar^3 w_{ik} \rho u^2} \quad \exp(-2\alpha k w_{ik}) \quad I_{ij}^{kl}\, \theta(E_{ik}-E_{jl}) \tag{15}$$

The transfer of momentum is also sufficiently small that this scattering can be considered quasi elastic. The deformation potential for such scattering is Ξ_h. The polar optical phonons in the oxide, the ionised impurities in the channel and acoustic phonons also interact with the holes at rates given by Eqs. (9), (13) and (14) respectively.

4 CARRIER MOBILITIES

The total scattering rate for an electron (hole) of momentum $\underline{k}$ or energy E relative to the bottom (top) of the band is

$$\lambda(E) = \sum_{\kappa} \lambda_{\kappa} \tag{16}$$

with κ = representing the individual scattering mechanisms and the expressions for λ_{κ} have been given in the previous section.

The total mobility of carriers in subband k of ladder i is

$$\mu_{ik} = e \langle\tau\rangle / m \tag{17}$$

where the average flight time $\langle\tau\rangle$ is assumed to be

$$1/\langle\tau\rangle = \int_{0}^{\infty} dE \; f(E+E_{ik})\lambda(E) \; . \tag{18}$$

This formula is strictly valid only for elastic scattering [14]. Monte Carlo particle simulation is being carried out to verify the justification of this assumption.

The drift velocity of carriers in subband k of ladder i is

$$v_{ik} = F\mu_{ik} \tag{19}$$

with F representing the longitudinal constant electric field. The total drift velocity v is

$$v = \sum_{ik} v_{ik} n_{ik} = F \sum_{ik} \mu_{ik} n_{ik} \tag{20}$$

with n_{ik} representing the occupancy of subband k of ladder i, given by Eq (6). The total mobility is:

$$\mu = \sum_{ik} \mu_{ik} n_{ik} \tag{21}$$

5 COMPARISON WITH EXPERIMENTAL DATA

The electron and hole mobilities have been measured versus the effective transversal field [15]. The relationship between the effective field F_e and the interface field, F_s, is

$$F_e = \gamma F_s + (1-\gamma) e \, N_{depl} / (\varepsilon \varepsilon_o) \tag{22}$$

where γ = 0.5 for electrons and 0.41 for holes. Figure 2 shows the measured mobilities versus F_s. The mobility has been measured against the effective field [15], and converted to the transversal interface field. The implanted impurity concentration, which is 5×10^{21} m^{-3} for the n-type

semiconductor and 7×10^{20} m^{-3} for the p-type one, respectively, is sufficiently small that the ionised impurity scattering can be neglected.

To compare the theoretical variation of mobility with that measured, values of the attenuation factor, α, and the deformation potentials Ξ are required. All deformation potentials are obtained by a common scaling factor from their bulk values. This scaling factor and α are then chosen to obtain agreement at both high and low surface fields. The agreement can be seen in Figure 2.

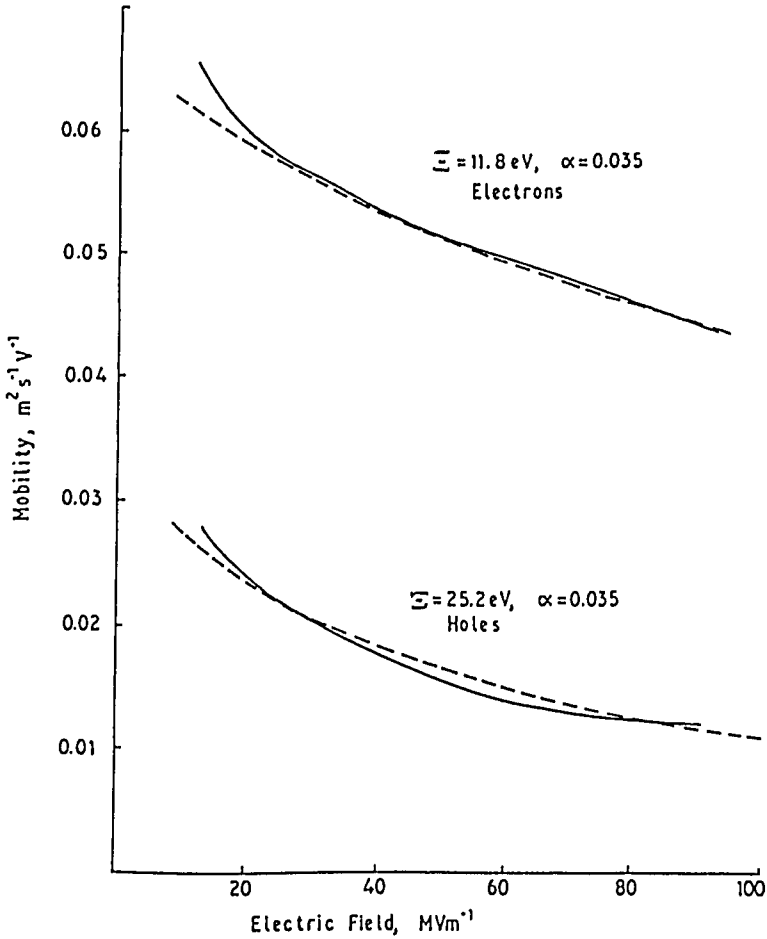

Figure 2: The calculated and measured mobilities of holes and electrons versus the perpendicular electric field.

The mobility for holes is not sensitive to α so that a reliable estimate of α cannot be obtained. The electron value has therefore been used. The theoretical curve has been calculated with the values indicated in the figure. Both for

holes and electrons the agreement between the measured and the calculated mobility is good, except at low fields, close to threshold. The low value of α indicates that the carriers feel the surfons almost unattenuated.

Figure 3 shows the calculated and measured mobilities versus temperature between 200 and 400 K, for an interface field of $F_s = 20\ MVm^{-1}$. The agreement for electrons is good above 270 K, below the theory overestimates the mobility. As ionised impurity scattering has been excluded from these calculations, this could explain some of the discrepancy, as this increases in importance as the phonon population reduces with the temperature.

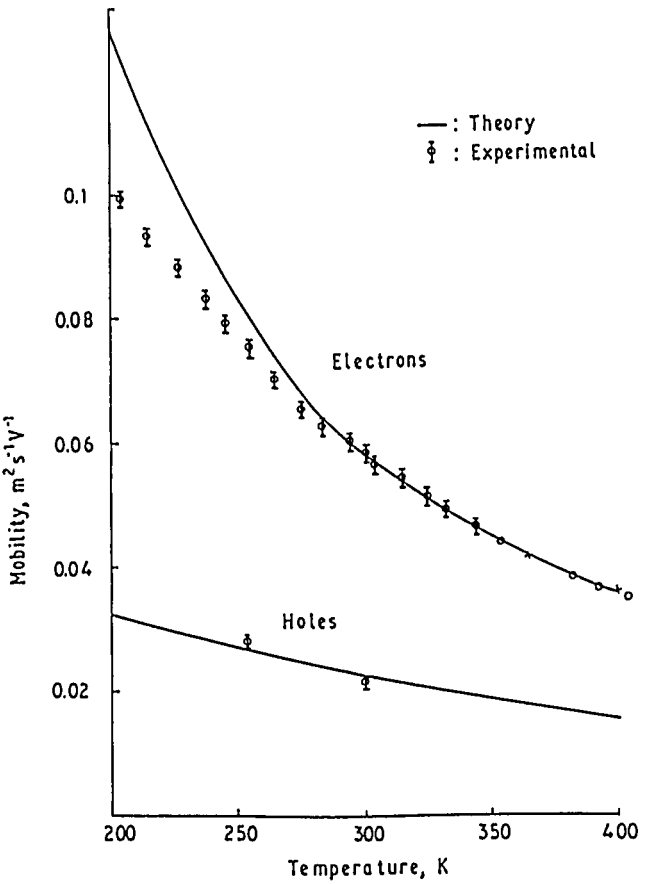

Figure 3: The calculated and measured mobilities of holes and electrons versus the temperature.

For holes the theory underestimates the mobility below room temperature and overestimates it above. The theory is

thus not as successful here. It is possible that an additional scattering mechanism, viz. second order surfons caused by optical phonons in the semiconductor should be included. From crystal symmetry arguments, optical phonons cannot interact with the carriers, but as the holes move away from the centre of the zone, the optical phonons can contribute to the scattering [11]. This is being investigated.

The measurements behind Figs 2 and 3 have been carried out on samples sufficiently pure that ionised impurity scattering should be negligible. The theoretical curves, too, have been calculated without it. Fig 4 shows the theoretical mobility versus the bulk doping density for both holes and electrons at room temperature and at an interface field of 20 MVm^{-1}. The effect of the ionised impurities start to be felt for doping around 10^{22} m^{-3}. From Eq (14) one reads that the ionised impurity scattering will contribute more at lower perpendicular fields becuase the width w_{ik} increases with decreasing field.

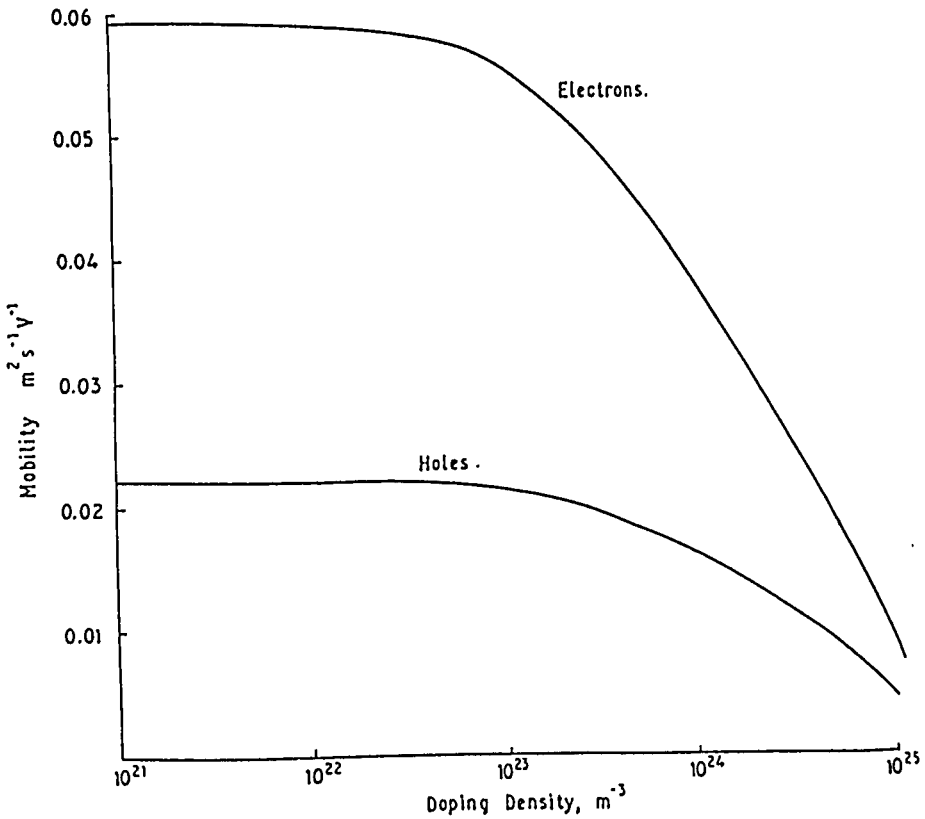

Figure 4: The calculated mobilities for holes in n-type and electrons in p-type silicon versus the uniform doping density.

6 CONCLUSION

The theory for the mobility of holes and electrons in the inversion layer interfaces, as formed at the gate in MOSFETs, has been re-examined in light of scattering of surfons from phonons and ionised impurities. The carriers move in a quantum well whose shape has been calculated by a self consistent solution of Schrödinger's and Poisson's equations, assuming that the subband population obeys Fermi-Dirac statistics. The effect on the mobility due to surfons decaying into the bulk is very weak. Ionised impurities do not play any significant role at room temperature for doping concentrations below 10^{22} m^{-3}. While the theory describes the measured mobility for the holes well, the temperature dependence of the mobility of the holes has not been correctly reproduced. There is room for a possible improvement by including second order scattering from optical phonons.

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