An analytical expression for phonon-limited electron mobility in silicon-inversion layers

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A complete Monte Carlo study of phonon-limited electron mobility in (100) silicon-inversion layers has been carried out. It has been determined advantageous to consider more than three energy subbands for electron motion. First-order intervalley scattering has also been shown to play an important role in ohmic transport. The results of the Monte Carlo simulation can be fitted by a simple analytical expression that coincides with the phonon-limited mobility for the bulk in the zero transverse-electric-field limit.

I. INTRODUCTION

Although widely studied, the limitation of electron mobility imposed by lattice vibrations in the inversion layers of metal-oxide-semiconductor structures is still not fully resolved.[1–3] The solution of this problem is of interest, among other reasons, to incorporate it in transistor modeling. For practical applications, it would be desirable to have a compact expression for the phonon-limited electron mobility, μ_{ph}, in order to include it in physical-based semiempirical models. This compact expression could be obtained by fitting experimental results, but it is difficult to obtain these data. Experimentally, some authors have tried to isolate μ_{ph} from the other mechanisms by considering this component not to contribute at all at 4.2 K and by applying the Matthiessen rule, according to which[4] $\mu_{ph}^{-1}(T)=\mu^{-1}(T)-\mu^{-1}(4.2\ \mathrm{K})$. However, this method could lead to misleading results because the rest of the mechanisms depend on temperature. Furthermore, the Matthiessen rule is not accurate at high and intermediate temperatures.[5] Due to these difficulties, an appropriate method for obtaining μ_{ph}, can be the detailed Monte Carlo simulation of electron transport.

In this article, we present the main results of a careful Monte Carlo simulation of the electron dynamics in *n*-Si (100) inversion layers, in which we have only considered phonon scattering.

II. METHOD

The mobility has been obtained by calculating the mean velocity along the inversion layer for several values of the longitudinal electric field and extrapolating to zero. We have chosen the lowest range of the longitudinal field that allows the calculation without excessive noise. We have studied the dependence of μ_{ph} on the mean transverse-electric field supported by the electron in the inversion layer, named E_{EFF} (defined in Ref. 6), in the range 5×10^4–10^6 V/cm. We have also looked into the dependence of μ_{ph} on the doping concentration of the substrate and on the temperature in the range 50–400 K. Details of the simulation and some results are discussed below:

(a) We have considered that the electrons in the inversion layer constitute a two-dimensional electron gas confined in a potential well at the interface. In these conditions the degeneracy of the six equivalent minima of the conduction band breaks and the electrons are distributed in two sets of subbands.[7] To obtain the effective transverse-electric field and the energy of the subbands for each value of the surface potential, we have self-consistently solved the Schrödinger and Poisson equations.[8] Except at very low temperatures or very high transverse-electric fields, it is not realistic to assume that most of the electrons are in the ground subband.[9] The occupation of higher subbands forces us to include the contribution of several subbands in the transport and to allow transitions among them. In these conditions, phonons mainly cause one of two types of electron transitions:[1] (a) intravalley acoustic transitions and (b) intervalley optical transitions, both of which have been adapted from their treatment in silicon bulk[10] to use them in Si(100) inversion layers. The scattering probabilities of these mechanisms have been deduced from the matrix elements for scattering of electrons by bulk phonons,[11,12] with the condition that the final state of the scattered electron must fall within an energy subband[1,13] and taking into account that the proximity of the interface could modify the coupling constants. The coupling constants, deformation potential, and phonon temperatures have been taken from Ref. 9. The use of bulk phonons is justified because the centroid of the electron distribution is placed at some distance from the interface. Other theoretical studies have used surface phonons or "surfons"[2,14] to characterize μ_{ph} versus the transverse-electric field, the temperature, and the doping concentration, but they have not been able to reproduce either the magnitude or the expected dependencies.[15]

(b) We have studied the effects of the number of subbands in the simulation. Although some authors have considered that it is an acceptable approximation to suppose that most of the electrons are in the lowest three subbands,[9] we have observed appreciable differences when considering a greater number. We therefore decided to allow the electron to move in six subbands in our Monte Carlo calculation even though we have considered twenty subbands for the solution of the Poisson and Schrödinger

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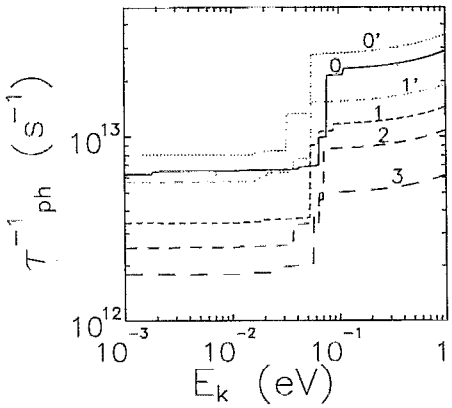

FIG. 1. Scattering rate for electrons in the lowest six subbands plotted vs the kinetic energy. Curves 0, 1, 2, 3 correspond to the twofold degenerate valleys whose longitudinal mass is in the direction perpendicular to the interface, and curves 0′, 1′ are for the fourfold degenerate valleys with longitudinal mass parallel to the interface ($E_{EFF}=7\times10^4$ V/cm, $T=300$ K).

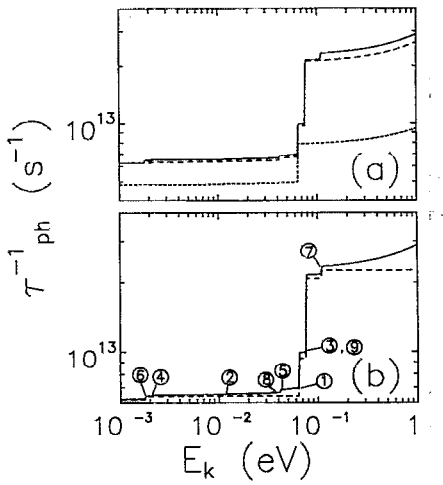

FIG. 2. Scattering rate for the electrons in the ground subband. In both (a) and (b), the total scattering rate obtained when electrons are allowed to move in six subbands is plotted (solid line). (a) shows the scattering rate for electrons when they are only allowed to move in the lowest three subbands (— — — —), or in the lowest subband (- - - - - - - -). (b) shows the scattering rate when considering only zero-order coupling (dashed line). Different phonon-assisted transitions are numbered here, as well. ($E_{EFF}=7\times10^4$ V/cm, $T=300$ K).

equations. For transverse-electric fields lower than the fields considered in this study, six subbands would also be insufficient. Nevertheless, in a complete simulation, mobility would be dominated by coulomb scattering due to the oxide and interface charges in the very low field region and practical interest in this field region would thereby be reduced. If coulomb scattering is strong, the three-subband approximation is also reasonable from a practical point of view.

(c) We have considered interactions both in zero and first-coupling order. The low-energy intervalley phonons considered in the model are forbidden in zero order,[16] so they have been treated via first-order interaction.[13] The first-order intervalley scattering has been shown to play an important role in hot-electron transport in silicon-inversion layers;[17] our results show that this mechanism is also important in ohmic transport.

The scattering rate for electrons in the lowest six subbands versus the kinetic energy, at 300 K, is plotted in Fig. 1. The steps that appear in the curves are produced when the electrons have enough energy to emit or absorb optical phonons moving to another subband or to emit optical phonons remaining in the same subband. These transitions are detailed for electrons in the ground subband in Fig. 2, wherein we also show the total scattering rate (solid line). The different phonon-assisted transitions are numbered as follows:

(1) Emission of a high-energy phonon (zero order, g type) with the electron remaining in subband E_0. The absorption of one of these phonons does not produce a step in the scattering rate.

(2) Emission of a low-energy phonon (first order, g type) with the electron remaining in subband E_0. The absorption does not produce a step in this case, either.

(3) Emission of a high-energy phonon (zero order, f type) with the electron moving to subband E_0'. The absorption does not produce a step in the scattering rate because the phonon energy is greater than the difference between the two subband minima.

(4) Absorption of a low-energy phonon (first order, f type) with the electron moving to subband E_0'.

(5) Emission of a low energy phonon with the electron moving to subband E_0'.

(6) and (7) Absorption and emission, respectively, of a high-energy phonon (zero order, f type), with the electron moving to subband E_1'.

(8) and (9) Absorption and emission, respectively, of a low-energy phonon (first order, f type), with the electron moving to subband E_1'.

Transitions from E_0 to E_1, E_2 or E_3 are forbidden in this model although they would be allowed in others.[18]

In Fig. 2(a) the results from allowing the electrons to move in six subbands is shown. We have also plotted the lower scattering rate that would be obtained if the electrons could move only in the ground subband (dotted line) or in the three lowest subbands (dashed line). With just one subband, only transition 1 occurs, while with three subbands transitions 1, 2, 3, 4 and 5 take place. In Fig. 2(b) the total scattering rate is compared with that which would be obtained by considering only zero-order coupling (dashed line). In this case only transitions 1, 3, 6, and 7 are allowed. It may also be observed from Fig. 2 (solid line) that the scattering rate increases linearly with regard to the energy due to the first-order coupling.

III. RESULTS

We have obtained mobility curves with different approximations to investigate the validity of the model described above. Figure 3 shows mobility curves obtained by allowing the electron to move in: (a) only the ground sub-

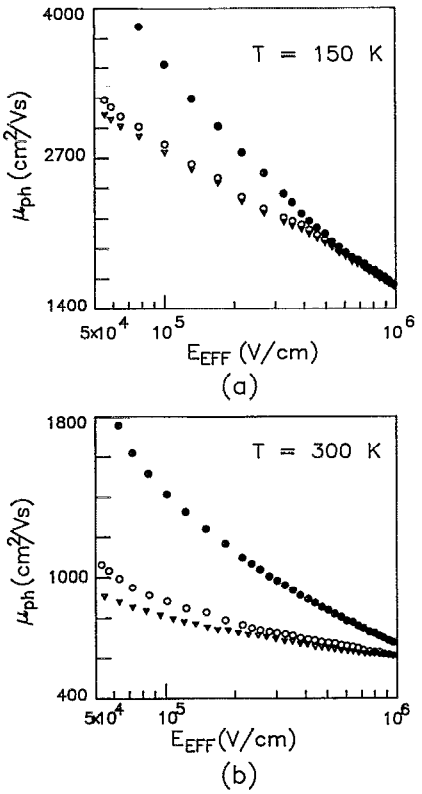

FIG. 3. Phonon-limited mobility of the electrons in a silicon-inversion layer vs the effective transverse-electric field. The effects of the number of subbands taken into account in the Monte Carlo simulation of parallel-electron transport is shown. (a) and (b) correspond to $T=150$ K and $T=300$ K, respectively. Data have been obtained by allowing the electrons to move in one subband (closed circles), three subbands (triangles), or six subbands (open circles).

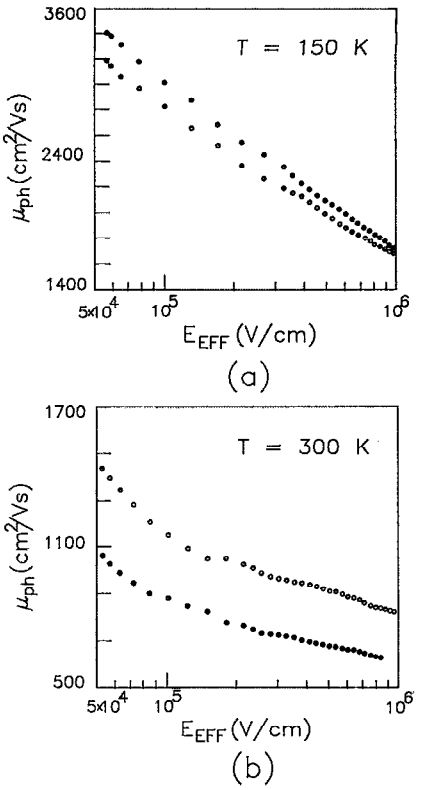

FIG. 4. Phonon-limited mobility of electrons in a silicon-inversion layer vs the effective-transverse-electric field. The effects of the first-order intervalley scattering are demonstrated. (a) and (b) correspond to $T=150$ K and $T=300$ K, respectively. Data have been obtained by including intravalley-acoustic scattering and optical-intervalley scattering. In data plotted with open circles, both zero- and first-order intervalley scattering are included, while in closed-circle data only zero-order intervalley scattering has been considered.

band, (b) the lowest three subbands, and (c) the lowest six subbands, all at different temperatures. The mobility with one subband is greater than with three subbands because in this case we allow the occupation of the lowest subband of the second set, where the effective mass is greater and mobility is lower. It can be seen that mobility with six subbands is higher than with three, and it can be also appreciated that the deviation is higher for lower electric fields or higher temperatures since the proportion of electrons contained in the higher subbands is greater. This is due to the lower scattering probability in the higher subbands of the same set.

Some mobility curves calculated for phonon scattering at $T=150$ K and $T=300$ K are given in Fig. 4 to show the effect of the first-order scattering. First-order intervalley scattering exerts a strong influence mainly at high temperatures where this scattering acquires importance. This emphasizes the desirability of including first-order intervalley scattering among the scattering mechanisms when a complete simulation of the mobility is done.

We have obtained curves of phonon-limited mobility with the model described for different temperature values in the range 50–400 K and different substrate doping. Our primary results have served as a check to validate our calculations. First, we have checked that the population of the different subbands, calculated from the mean time that the electron spends in them, coincides with the value calculated taking into account the difference between the Fermi level and the energy of the subbands. As well, the curves obtained for different substrate doping concentrations in the range $N_A=10^{13}$–10^{18} cm^{-3}, at 300 K, are superposed. This confirms the universal behavior of the mobility versus E_{EFF}, observed experimentally by Sabnis and Clemens.[6] The results obtained for three different temperatures and for a doping concentration of $N_A=10^{16}$ cm^{-3} are shown in Fig. 5 (symbols). For very low transverse-electric fields, the occupation of higher subbands is important and the electron gas is less confined.[19] In consequence, the electron gas tends to be three dimensional and μ_{ph} must approach the bulk value in the $E_{EFF}=0$ limit. Therefore, basing ourselves on the following model:

$$\frac{1}{\mu_{ph}(T)}=\frac{1}{\mu_{phB}(T)}\left[1+\beta(T)E_{EFF}^{\alpha(T)}\right], \tag{1}$$

where $\mu_{phB}(T)$ is the phonon-limited mobility in the bulk (from Ref. 20), we have proposed:

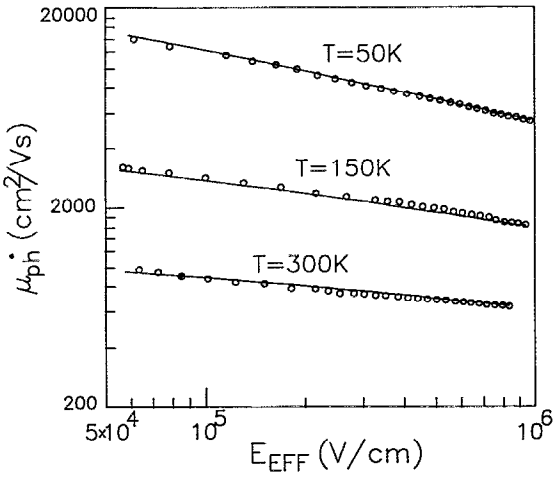

FIG. 5. Phonon-limited mobility of electrons in a silicon-inversion layer vs the effective-transverse-electric field obtained by a complete Monte Carlo simulation of the electron transport, at different temperatures (circles). Solid-line curves correspond to an empirical model based on an analytical expression. Excellent agreement can be noted.

$$\frac{1}{\mu_{\rm ph}(T)}=\frac{1}{\mu_{\rm phB}(300{\rm K})}\left[\left(\frac{T}{300{\rm K}}\right)^{n}+\left(\frac{T}{300{\rm K}}\right)^{r}\left(\frac{E_{\rm EFF}}{E_0}\right)^{\alpha(T)}\right], \tag{2}$$

where $T=300$ K is taken as a reference.

This Monte Carlo results fit expression (2) with a deviation lower than $\pm 5\%$. We have used $\mu_{\rm phB}=1470$ cm^2 V^{-1} s^{-1} and $n=2.109$; the best adjustment was obtained with $r=1.003$, $E_0=3.588\times10^5$ V/cm and $\alpha(T)=0.325\times(T/300\ {\rm K})^{-0.13}$. The curves corresponding to the model are also shown in Fig. 5 (solid line).

A comparison of the results of our calculation to experimental results is shown in Fig. 6. The experimental mobility curves (symbols) have been obtained from the drain current versus gate voltage in the linear region of an n-channel MOSFET, at different temperatures and for different concentrations of the oxide charge. Besides phonon scattering (considered in this article) other mechanisms such as coulomb and surface-roughness scattering are also present. Experimental curves in Fig. 6 correspond to a transverse electric field where $E_{\rm EFF}=1.8\times10^5$ V/cm. We have chosen an intermediate value neither so high that surface roughness dominates nor so low that phonon scattering would be completely masked by coulomb scattering. The lower the oxide charge, the weaker the coulomb scattering and the higher the mobility. At the limit of zero

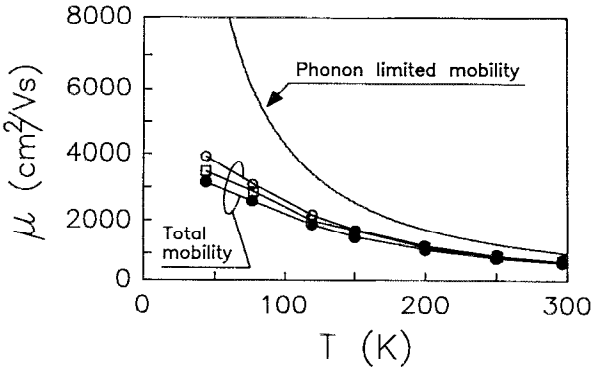

FIG. 6. Comparison of calculated phonon limited mobility (solid line) and experimental results (symbols) for a transverse electric field where $E_{\rm EFF}=1.8\times10^5$ V/cm. In experimental results, other inevitable scattering mechanisms are present besides phonon scattering. Curves for three different oxide charges are shown: (○) $N_{\rm ox}=4.0\times10^{10}$ cm^{-2}, (□) $N_{\rm ox}=7.4\times10^{10}$ cm^{-2}, (●) $N_{\rm ox}=8.9\times10^{10}$ cm^{-2}.

coulomb and surface-roughness scattering, experimental curves must approach our theoretical results (Fig. 6, solid line).

IV. CONCLUSIONS

We have obtained an analytical expression for the component of the electron mobility limited by phonons in Si(100)-inversion layers. We have seen that it is advantageous to consider more than three energy subbands for the electron motion, and have determined that six subbands is an appropriate number for the range of transverse-electric fields treated in this study. The first-order intervalley scattering also plays an important role in ohmic transport.

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