Explaining the Dependences of Electron and Hole Mobilities in Si MOSFET's Inversion Layer

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Abstract

In this paper we report a detailed study of the surface roughness (SR) limited mobility and, for the first time, a physical explanation of the different dependences of the electron and hole mobilities. Based on full-band Monte Carlo simulations, we show that the differences between hole and electron experimental mobilities can be accounted for by using a steeper tail of the SR power spectrum at high wavevector values. The new power spectral density allows to fit all the experimental data at room and cryogenic temperature, with the same parameter values for both electrons and holes. The spatial dependence of the new SR spectrum is discussed and compared to the features of the SR described by exponential and gaussian auto-covariance functions.

Introduction

Despite the dominant scattering mechanisms in Si inversion layer have long been studied, there are still some peculiar differences between electron and hole mobilities that have to be clarified. It is well established that the mobility curves are *universal*, that is independent of channel doping, if they are plotted as a function of the transverse effective electric field $E_{eff} = (Q_d + \eta Q_{inv})/\epsilon_{Si}$, where η is a coefficient empirically taken as 1/2 for electrons and 1/3 for holes (1, 2). Increasing the effective field and pushing the carriers against the Si/SiO_2 interface, the low temperature electron mobility degrades as E_{eff}^{-2} while the hole mobility follows the E_{eff}^{-1} power law (2).

In our work carriers mobilities have been computed relying on a full-band Monte Carlo (MC) code and on an equivalent effective mass model. In order to handle the bias dependence of the valence band (3), the MC has been coupled to a detailed band-structure calculation obtained solving self-consistently the one-dimensional Poisson equation and the Schrödinger equation with a 6-band $\mathbf{k}\cdot\mathbf{p}$ procedure (4). Moreover, updated models of the scattering (4) and of the carrier screening have been included (5). Following (6), the SR scattering is described by a potential perturbing the carrier transport with a power spectral density $S(q)$, the latter being the Fourier transform of the auto-covariance function of the spatial features of the Si/SiO_2 interface. The auto-covariance shape has been so far taken either gaussian or exponential (7). For the gaussian spectrum, it is:

$$S(q) = \pi \Delta^2 \Lambda^2 e^{-\frac{(q\Lambda)^2}{4}} \tag{1}$$

where Δ is the roughness r.m.s. value and Λ is the correlation length. However, by using these functional dependences there is no way to find a single $S(q)$ shape accounting for both electron and hole data. Figs. 1 and 2 show the comparison between data and simulation results by taking $S(q)$ gaussian with parameters adjusted to fit the electron mobility curves (Δ = 2.7 Å and Λ = 10.3 Å). Since the SR-limited mobility is dominant at low temperature, the figures report experimental and calculated data at 77 K. Figs. 3 and 4 show the opposite, i.e. the gaussian $S(q)$ accounting for the hole mobility does not fit the electron data (Δ = 1.9 Å and Λ = 20.5 Å). Similar results have been obtained adopting the exponential auto-covariance function and tailoring its parameters.

The discrepancy has been solved by observing that the holes reach k values higher than electrons and therefore they are more sensitive to the high-k region of the SR spectrum. It is known that mobility is limited by the scattering of the carriers close to the Fermi energy. At low temperatures the k-wavevector of these carriers is approximatively given by $k_F = \sqrt{2\pi N_s/g_\nu}$, where N_s is the carrier density and g_ν is the degeneration factor. Since $g_\nu = 2$ for the electrons, while most of the holes lie in the heavy-hole band, the electron k-wavevector is expected to be always lower than that of the holes, when compared at the same carrier density N_s. The same result holds true also at higher temperature. Fig. 5 shows the dependence on N_s of the k-wavevector of the carriers mainly contributing to the momentum relaxation time as numer-

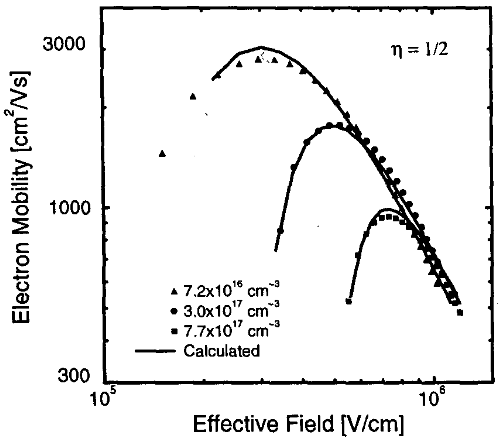

Figure 1: Experimental electron mobility (1) at 77 K and SR-limited mobility computed using a gaussian power spectral density with $\Delta = 2.7$ Å and $\Lambda = 10.3$ Å.

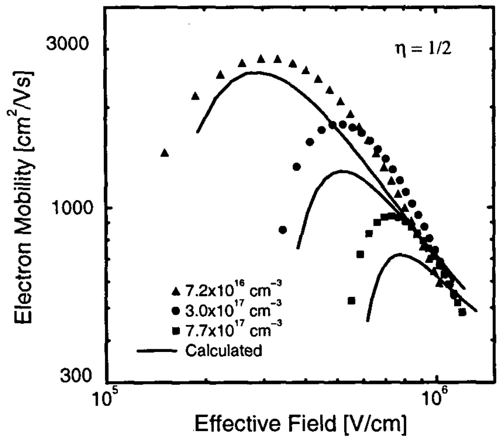

Figure 3: Experimental electron mobility at 77 K and SR-limited mobility computed using a gaussian power spectral density with $\Delta = 1.9$ Å and $\Lambda = 20.5$ Å.

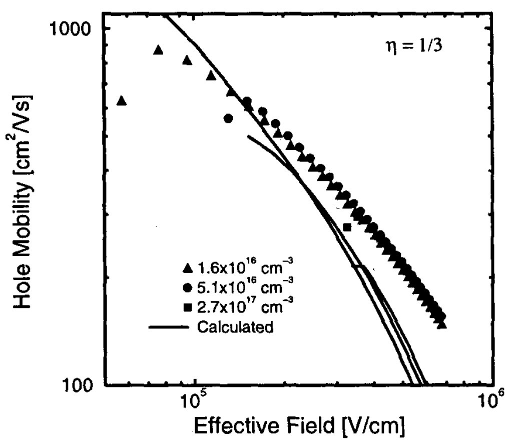

Figure 2: Experimental hole mobility (1) at 77 K and SR-limited mobility computed using a gaussian power spectral density with $\Delta = 2.7$ Å and $\Lambda = 10.3$ Å.

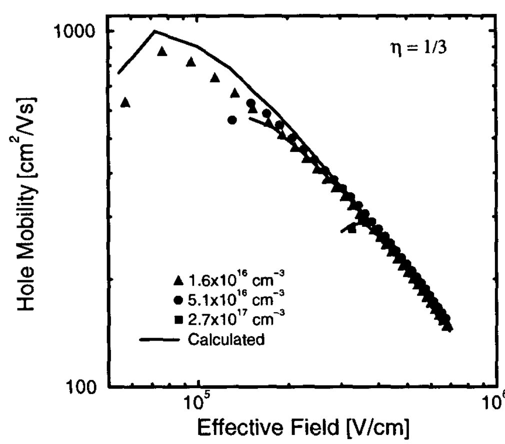

Figure 4: Experimental hole mobility at 77 K and SR-limited mobility computed using a gaussian power spectral density with $n = 2$, $\Delta = 1.9$ Å and $\Lambda = 20.5$ Å.

ically computed. At 77 K this k value is close to k_F. At 300 K it is instead higher than k_F, due to the contribution of the thermal energy. In any case the holes reach higher k values than electrons.

A New Model for the Power Spectrum

It turns out that a roughness power spectrum that may account for both electron and hole data should be similar, in the low-k region, to the gaussian function fitting the electron mobility, while in the high-k region it can be properly tailored to match the hole data. The new $S(q)$ was therefore taken as:

$$S\left(q\right) = \pi \Delta^2 \Lambda^2 e^{-\frac{(q\Lambda)^n}{4}}. \qquad (2)$$

For $n = 2$ it reduces to the gaussian shape, while as n is increased the low-k region remains almost the same and the $S\left(q\right)$ high-k tail is cut off (Fig. 6). By changing n only the hole mobility is affected, leaving the electron mobility almost unchanged. By taking $n = 4$, $\Delta = 2.7$ Å and $\Lambda = 10.3$ Å the universality of the hole mobility is recovered (Fig. 7) and the same SR parameters are able to

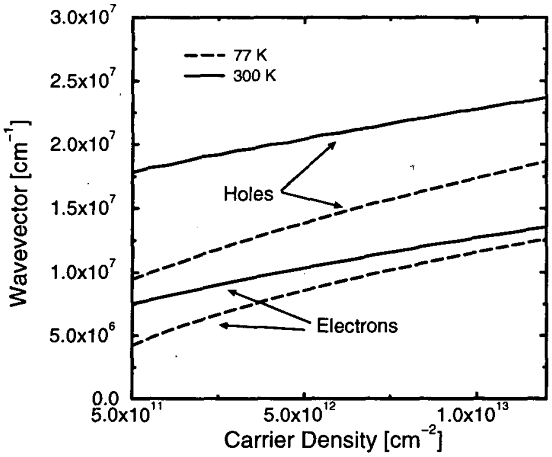

Figure 5: k-wavevector of the electrons and holes that mainly contributes to the SR-limited mobility at 77 K (dashed lines) and 300 K (solid lines).

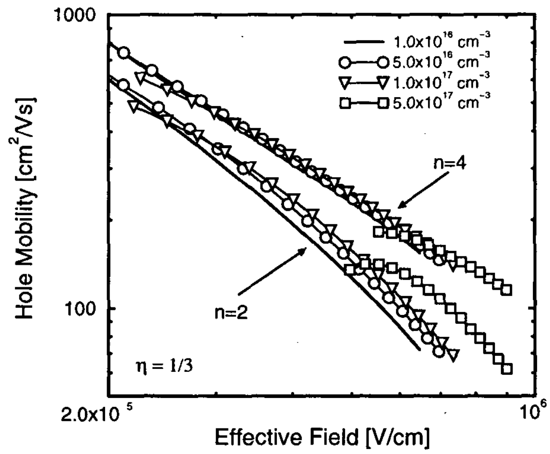

Figure 7: Hole SR-limited mobility at 77 K computed using power spectral densities with $n = 2$ and $n = 4$ ($\Delta = 2.7$ Å and $\Lambda = 10.3$ Å).

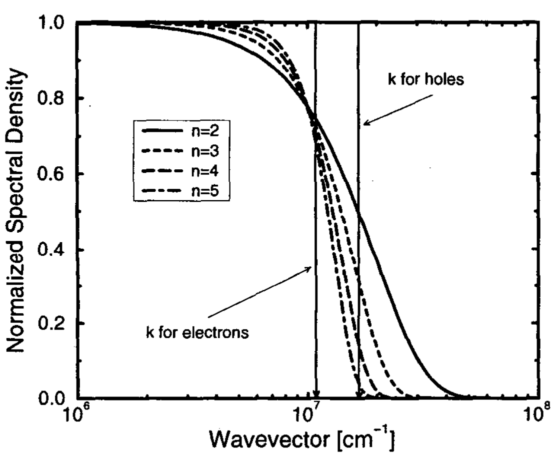

Figure 6: Power spectral densities obtained from (2) by changing the n value. The vertical lines highlight the upper spatial frequencies of the power spectrum contributing to the SR-limited mobility of electrons and holes, respectively, when $N_s = 10^{13}$ cm^{-2}.

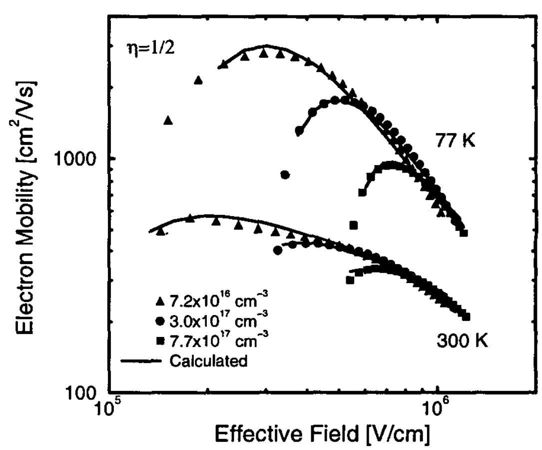

Figure 8: Experimental values of the electron effective mobility at 77 K and 300 K (symbols). They are plotted as a function of the effective field with $\eta = 1/2$. The solid lines show the effective mobility computed using (2) with $n = 4$, $\Delta = 2.7$ Å and $\Lambda = 10.3$ Å.

fit both the electron and the hole mobilities (Figs. 8 and 9) at room temperature and 77 K. These results demonstrate that the different η values in the E_{eff} definition and the different power law degradation at high E_{eff} can be explained within the known theoretical framework. As reported in (3) these features are not due to the valence band anisotropy. We have shown instead that they can result from the shape of the SR power spectrum at high k-values.

The spatial features of the roughness at the Si/SiO_2 interface have been investigated with TEM (7) and AFM (8) techniques. Although not conclusive these results suggest that the interface is uneven on the spatial scale of a few atomic steps at least. Fig. 10 compares the surface structure described by (2) with $n = 4$ to

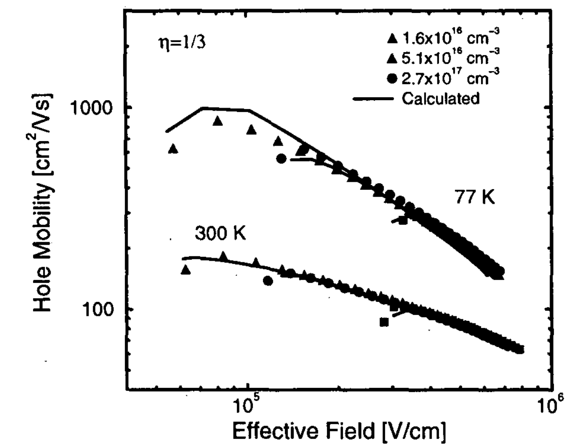

Figure 9: Experimental values of the hole effective mobility at 77 K and 300 K (symbols). They are plotted as a function of the effective field with $\eta = 1/3$. The solid lines show the effective mobility computed using (2) with $n = 4$, $\Delta = 2.7$ Å and $\Lambda = 10.3$ Å.

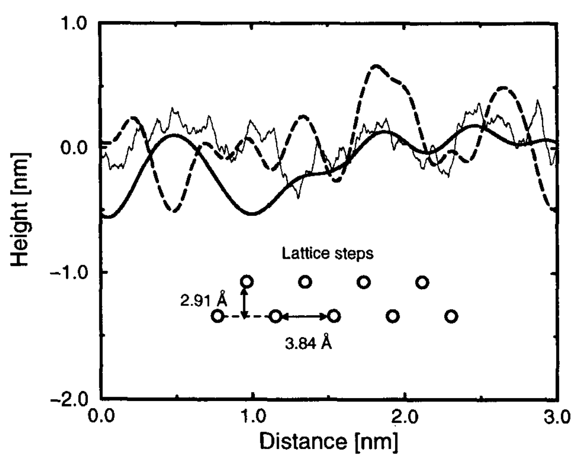

Figure 10: Spatial features corresponding to the spectral approximation with $n = 4$ (solid line), $n = 2$ (dashed line) and exponential auto-covariance function (thin solid line). Circles point out the relevant dimensions of lattice steps.

those described by a gaussian $S(q)$ ($n = 2$) and by the exponential auto-covariance proposed in (7). Note that the latter gives rise to roughness with sharp variations and it seems therefore the least plausible. The gaussian spectrum describes a smoother interface. The new shape, with its cut off of the high-frequency components, describes a roughness even smoother. We may therefore conclude that, also from this standpoint, the shape given by (2) seems the most acceptable among the three.

Conclusions

The differences between electron and hole mobility have been investigated relying on full-band Monte Carlo calculations. We show that these differences are due to the physics of the SR scattering and we succeed in identifying a single power spectral density that makes possible to quantitatively account for both the experimental electron and hole mobilities.

References

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