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A Consistent Model for Low and High-Field Electron Transport in Homogeneous Silicon Inversion Layers†

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A microscopic transport model for the quasi 2D electron gas in a homogeneous inversion layer of a MOS-system is presented. The model relies on the discrete subband structure without artificially restricting the number of subbands. The dependence of the mobility on the electric field strength is modeled on the basis of three different types of scattering mechanisms taking into account Pauli's exclusion principle and the effect of nonparabolicity. Low and high-field mobilities resulting from this model are compared with measurements.

INTRODUCTION

Modeling MOSFET devices the evaluation of the electron mobility as a function of the electric field strength is very important. In particular, device characteristics are strongly influenced by the normal field dependence of the mobility in silicon inversion layers. Under the influence of an electric field applied normal to the SiO_2/Si-interface of a MOS-device the carriers in the inversion layer form a quasi two-dimensional (2D) electron gas because they are confined to a narrow potential well. Therefore, to get a deeper insight into the microscopic details of the transport behaviour of electrons in inversion layers the theoretical analysis must take this quantization of the electronic states into account. In this paper a transport model is presented, which includes the structure of the above mentioned discrete subband levels. It is shown that through this model the field dependence of the mobility under technical relevant operating conditions is reproduced. Since this paper is focused only on the principle mechanisms determining the transport properties of a quasi 2D electron gas, inversion layers are considered here, which are homogeneous in the directions parallel to SiO_2/Si-interface.

MODEL

The electronic wavefunctions perpendicular to the SiO_2/Si-interface are obtained by solving Schrödinger's and Poisson's equation self-consistently.[1] Based on these results the multisubband transport parallel to the SiO_2/Si-interface is described by a coupled system of non-linear Boltzmann transport equations considering Pauli's exclusion principle.[2] The collision term in each of these equations contains three scattering mechanisms – phonon scattering, impurity scattering, and surface roughness scattering.[3] To describe the interaction of the quasi 2D electron gas with the lattice vibrations it is possible to adopt the well accepted phonon model of C. Jacoboni et al.[4] by neglecting the modification of bulk phonon spectra due to the interface. In addition, using an elastic approximation for scattering due to long-wavelength acoustic phonons yields the expression for the transition probability derived by P.J. Price[5]. The principle difference between the surface and the bulk case is given by the dependence of the scattering rate on the overlap integral

$$\frac{1}{L^{(v',v)}_{(n'n)}} = \int_0^\infty dz \left|\xi^{(v')}_{n'}(z)\right|^2 \left|\xi^{(v)}_{n}(z)\right|^2 \qquad (1)$$

where $\xi^{(v)}_n(z)$ denotes the localized part of the electronic wavefunction in subband n of valley v. The acoustic phonons with long wavelength can induce intravalley intrasubband and intravalley intersubband transitions. It is worth to mention that only in the case of the electric quantum limit the value of the overlap integral is proportional to $N_{inv}^{-1/3}$. However, in general this result is not valid.

The intervalley transitions are described via zero-order phonon coupling involving three f- and three g-type phonons. Generalizing Price's treatment[6] the scattering rate is derived leading to an expression which is also proportional to the overlap integral (1). In contrast to earlier works[7,8] this derivation of the scattering rate shows that both intrasubband and intersubband transitions are possible due to intervalley phonons. The deformation

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potentials of these intervalley phonons are chosen to be the same as in C. Jacoboni's bulk model[4] while the coupling constant of the long-wavelength acoustic phonons has to be increased in order to reproduce experimental results. This stronger coupling of phonons and electrons in the inversion layer can be explained by the interfacial stress.

Scattering of electrons by surface roughness is described following the treatment by Y.C. Cheng[9]. The surface asperities are modeled by an Gaussian autocorrelation function containing two parameters. Since these parameters can not be directly measured with sufficient precision they have to be chosen in a reasonable range in accordance with experiments. The resulting scattering rate is proportional to the square of the matrix element

$$M_{n'n}^{(v)} = \int_0^\infty dz \{\xi_{n'}^{(v)}(z)\}^* E(z) \xi_n^{(v)}(z) \qquad (2)$$

where the function $E(z)$ represents the electric field strength in the channel perpendicular to the SiO_2/Si-interface. If only one subband is occupied by electrons, this matrix element equals the effective electric field strength[10] given by $E_{eff} = \frac{e}{\epsilon_{si}}(N_{depl} + \frac{1}{2}N_{inv})$. However, if more than one subband is occupied, no such simple relation between the value of the matrix element (2) and E_{eff} can be expected. Moreover, screening significantly modifies the dependence of surface roughness scattering on the electric field strength as shown by S. Mori[11]. Scattering by surface charges and bulk impurities is modeled taking into account the full $\vec{q}$-dependence of the screened matrix elements[2,6] where $\vec{q}$ denotes the momentum exchange between the two-dimensional wavevector of the final and the initial electron state. Both, surface roughness and impurity scattering induce only transitions between electronic state within the same valley.

Two different methods are used to solve the coupled set of Boltzmann transport equations, namely the Monte Carlo approach and the relaxation time approximation. While the Monte Carlo method is valid over the full range of driving fields E_{tang} parallel to the SiO_2/Si-interface, the relaxation time approximation is limited to the linear transport regime. However, since both methods yield the same results for the low-field mobility ($E_{tang} \leq 1\,kV/cm$), it is possible under linear transport conditions to choose the relaxation time approximation which reduces the computational effort by several orders of magnitudes. Pauli's exclusion principle is included in both methods.[12,13] Furthermore, the nonparabolicity of the lowest conduction-band is considered. This has been achieved by using the dispersion relation

$$\epsilon_{\vec{k}}^{(v)}\left[1 + \alpha\epsilon_{\vec{k}}^{(v)}\right] = \frac{\hbar^2}{2}\left(\frac{k_x^2}{m_x^{(v)}} + \frac{k_y^2}{m_y^{(v)}}\right) \qquad (3)$$

between the kinetic energy $\epsilon_{\vec{k}}^{(v)}$ and the components k_x, k_y of the two-dimensional wavevector $\vec{k}$ parallel to the SiO_2/Si-interface. Such a treatment can be motivated by a Taylor series expansion of the bulk dispersion relation in silicon neglecting the coupling between $\vec{k}$ and k_z.

RESULTS AND DISCUSSION

By solving Schrödinger's and Poisson's equation self-consistently the splitting of the lowest conduction-band into a system of subbands of different energy levels is determined. In *fig. 1* this splitting is shown as a function of channel doping. With increasing doping concentration the splitting of energy levels increases. The energy difference between the two lowest subbands is greater than the thermal energy K_BT of the electrons in the given range of doping concentrations. This indicates that modeling transport of carriers within the inversion layer quantum mechanical effects can not be neglected. Moreover, for an induced electron concentration per unit area of $5 \cdot 10^{12}\,cm^{-2}$, the energy of the lowest subband is located near the Fermi level E_F. Therefore, even at room temperature the consideration of Pauli's exclusion principle is mandatory at least in this subband.

For smaller induced electron concentrations the separation between energies of different subband levels decreases and the relative occupation of the higher subbands increases. Therefore, it is necessary to consider a sufficiently large number of subbands to model the transport behaviour of the system consistently to the density of states under weak inversion conditions. In *fig. 2* it is demonstrated, how an artificial limitation of the number of subbands influences the electron mobility in inversion layers. The comparison with experimental data[14] shows clearly that particularly in weak inversion the contribution of higher subbands is important. To appreciate the necessary number of subbands, here all levels with an energy E obeying the condition $E - E_F < 10K_BT$ are accounted to be relevant. This condition implies that

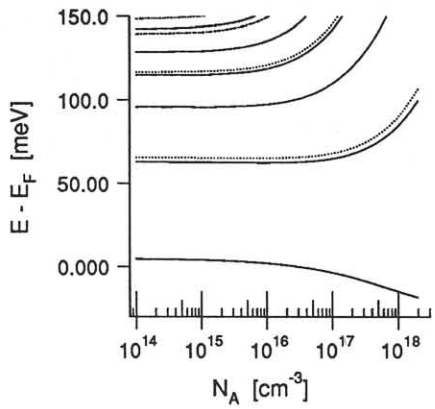

Fig. 1: subband splitting as a function of doping concentration for an induced electron density per unit area of $5 \cdot 10^{12}\,cm^{-2}$ at room temperature

the number of relevant subbands depends on the doping concentration of the silicon substrate. This dependence can also be estimated from *fig. 1*.

Figure 3 shows the low-field mobility μ as a function of the effective electric field E_{eff} for four different doping concentrations. As in *fig. 2* the experimental data have been taken from a work of J.A. Cooper and D.F. Nelson[14] who used a MOS-device with a doping concentration of $1.2 \cdot 10^{14}\,cm^{-3}$. Since the various curves and the experimental data deviate by less than 5% under

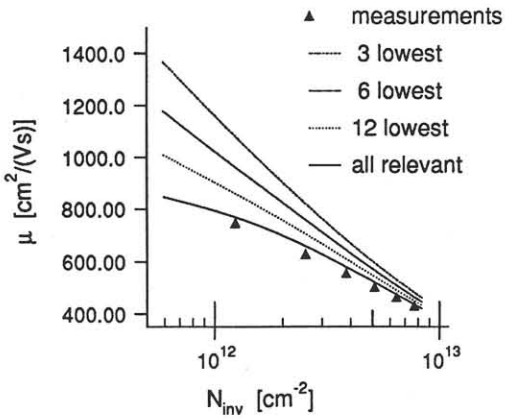

Fig. 2: low-field mobility for different numbers of considered subbands compared to experimental results

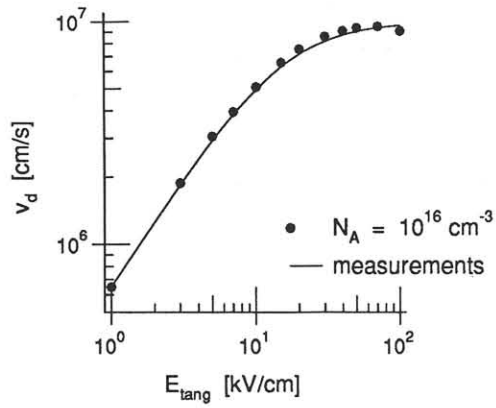

Fig. 4: drift velocity versus the tangential electric field strength in the inversion layer for an effective field strength of 200 kV/cm

strong inversion conditions the theoretical model is able to reproduce the universal relation between μ and E_{eff} found by A.G. Sabnis and J.T. Clemens[15]. The deviation of the curves from the universal relation for higher doping concentrations and weak inversion is attributed to a reduction of screening with decreasing induced electron density and an enhanced impurity scattering. It should be emphasized that the theoretical curves all rely on the same set of model parameters and the result has been achieved by only changing the doping concentration of the substrate. In order to explain the experimentally observed relation between the low-field mobility and the

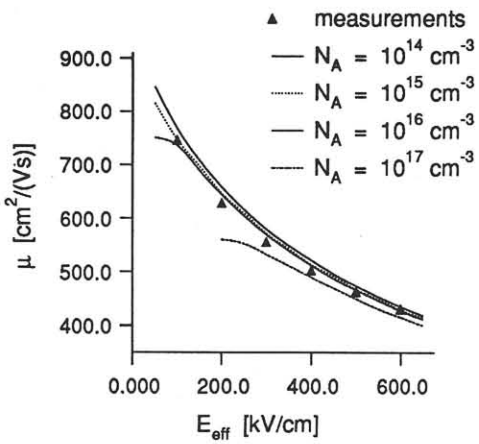

Fig. 3: dependence of the low-field mobility on the effective electric field strength for different doping concentrations

effective field strength over the whole range of fields it is necessary to take the joint effect of all three different kinds of scattering mechanisms into account.

A comparison of the drift velocity v_d resulting from Monte Carlo simulations with measurements[14] is shown in *fig. 4* as a function of the tangential electric field E_{tang} in the channel. Relying on the same set of model parameters used in the low-field case the dependence of v_d on E_{tang} as well as the magnitude of the saturation velocity can be described sufficiently accurate. It is worth mentioning that achieving such a good agreement between experimental data and theoretical results can only be obtained, if nonparabolicity is taken into account.

CONCLUSION

It has been demonstrated that considering quantum effects is mandatory for microscopically modeling the transport properties of electrons in silicon n-inversion layers especially for modern deep submicron MOS-devices with channel doping concentrations up to the order of $10^{18}\,cm^{-3}$. The good agreement between experimental data and theoretical results proves that at room temperature electron transport under low and high parallel field conditions can be described consistently with one model.

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