Simulation of Magnetotransport in Hole Inversion Layers Based on Full Subbands

A. T. Pham [a], C. Jungemann [b], and B. Meinerzhagen [a]
[a] BST, TU Braunschweig, Postfach 33 29, 38023 Braunschweig, Germany
e-mail: pham@nst.ing.tu-bs.de
[b] EIT4, Bundeswehr University, 85577 Neubiberg, Germany

Abstract

Magnetotransport of holes in Si inversion layers of 1D MOS capacitors on arbitrarily oriented substrates is simulated. The $6\times 6\ \vec{k}\cdot\vec{p}$ Schrödinger equation is solved self-consistently with the confining electrostatic potential to calculate the 2D hole gas subband structure. The transport of holes within the channel is investigated by solving the stationary Boltzmann equation (BTE) for a small lateral driving electric field. The distribution function is either expressed as a polynomial of the magnetic field or expanded into harmonics of the polar angle within 2D $\vec{k}$-space (Fourier expansion). The Hall factor and the second order magnetotransport coefficients are calculated. The approximation of the second order coefficient by the square of the channel mobility is shown to fail.

1 Introduction

Magnetotransport measurements can be used to characterize the inversion layer transport in MOSFETs [1, 2]. To this end the Hall factor or the second order coefficients, i.e. $-\frac{1}{2I}\frac{\partial^2 I}{\partial B^2}|_{B=0}$ (I: collector current or drain current, B: magnetic field) are usually measured. The simulation of magnetotransport in hole inversion layers for arbitrary magnetic field strengths based on the solution of the $\vec{k}\cdot\vec{p}$ Schrödinger, Poisson, and BTE is presented in this work.

2 Theory

The Hall factor and the second order coefficients are calculated for homogeneous inversion layers of 1D Si pMOS capacitors based on the solution of the stationary BTE. The quasi 2D hole gas subband structure with arbitrary surface orientation is calculated by solving the $6\times 6\ \vec{k}\cdot\vec{p}$ Schrödinger equation self-consistently with the confining electrostatic potential. The magnetic field of arbitrary field strength perpendicular to the substrate surface can be considered. The transport model includes scattering by phonons and surface roughness. The scattering integral is approximated with a relaxation time τ which depends on energy and subband index. The calculation of individual relaxation time for each scattering mechanism and of the total τ for all scattering mechanisms is described in [3]. Since the driving electric fields are small in magnetotransport measurements, the stationary BTE is linearized w.r.t. the driving electric field in channel direction [4]. The linearized BTE can be solved by expanding the distribution function

into a polynomial of B: $f(B) = g_{(0)} + g_{(1)}B + g_{(2)}B^2 + g_{(3)}B^3 + \ldots$ The component $g_{(n)}$ is recursively calculated from $g_{(n-1)}$. A problem of this expansion is that the microscopic inverse mass tensor (MIM) occurs in $g_{(1)}$ and its higher order derivatives in $g_{(2),(3),..}$. These high order derivatives are difficult to evaluate numerically.
In order to avoid these numerical problems a new method based on the Fourier expansion of the distribution function is used to solve the linearized BTE. This is the 2D $\vec{k}$ space analogue of the spherical harmonics expansion in 3D. It takes only a few CPU minutes to calculate the Fourier expansion coefficients for all energy levels and subbands.

3 Results

In Fig. 1 the simulated zero magnetic field mobilities of unstrained Si bulk pMOS transistors are shown, which reproduce the measurements from [5] for (100) and [6] for (110) surface orientations very well. The effective mass (Fig. 2) along the transport

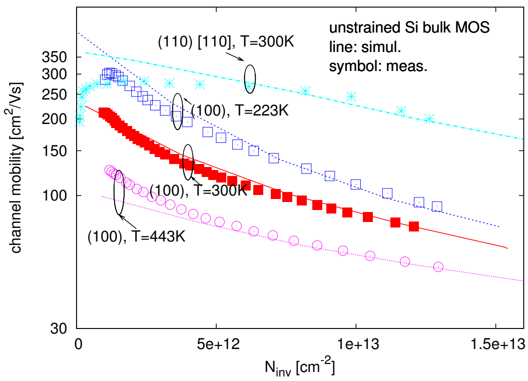

Figure 1: Zero magnetic field inversion layer mobility of unstrained Si bulk pMOS transistors. Measurements are taken from S. Takagi et al. [5] for (100) and H. Irie et al. [6] for (110) surface orientations.

direction for the (110) (interface) [110] (channel) configuration is much smaller than for the (100) substrates. For the (100) surface the response in [011] direction is similar to the response in [001] direction. Therefore only the [011] case is shown in this paper for the (100) surface. The change of the band structure and of the matrix elements of the scattering processes causes the increase of the Hall factor (Fig. 2) when changing from the (100) to the (110) [110] configuration. The second order coefficient (α) is plotted in Fig. 3. The Hall factor and α calculated for small magnetic fields by both, the polynomial and Fourier expansion methods, are in good agreement. The often used approximation for the second order coefficient $\alpha \approx \mu^2$ on the other hand causes a very large error. Fig. 4 shows the mobilities for strong magnetic fields. It can be seen that the polynomial expansion fails at higher magnetic fields. This is due to numerical errors in the MIM and its derivatives. In case of an analytic approximation for the subband dispersion relation this problem vanishes (Fig. 5).

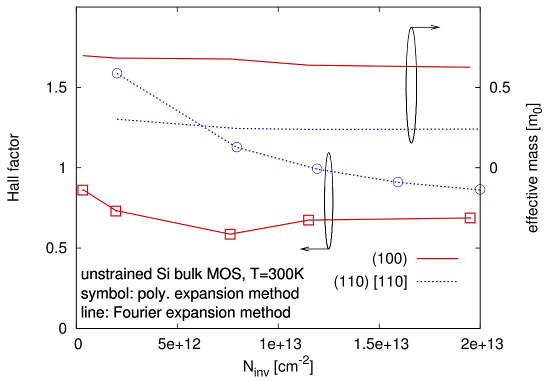

Figure 2: Effective mass in transport direction and Hall factor as function of the inversion density at room temperature.

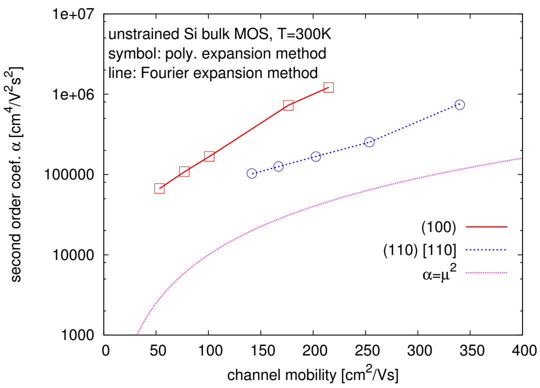

Figure 3: Second order coefficients including the approximation $\alpha \approx \mu^2$ as a function of the channel mobility.

4 Conclusion

The Hall factor and the second order coefficient have been calculated by a new Fourier expansion method. The approximation of the second order coefficient by the square of channel mobility is shown to fail. In the case of strong magnetic fields numerical problems occur in the case of the polynomial expansion, which are avoided by the new approach.

References

[1] W. Chaisantikulwat et al., "Magnetoresistance technique for mobility extraction in short channel FDSOI transistors," in *Proc. ESSDERC*, (Grenoble, France), pp. 569–572, 2005.
[2] J. Lusakowski et al., "Influence of ballistic and pocket effects on electron mobility in Si

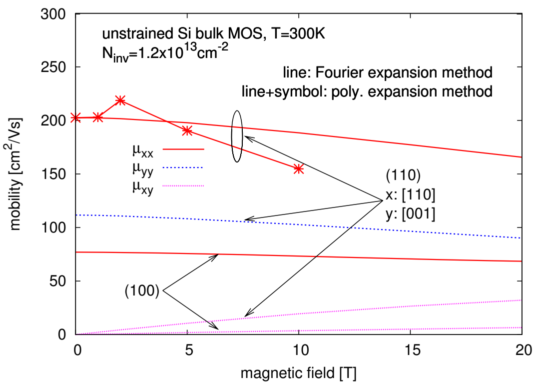

Figure 4: Mobilities as a function of the magnetic field calculated by the Fourier and polynomial expansion method.

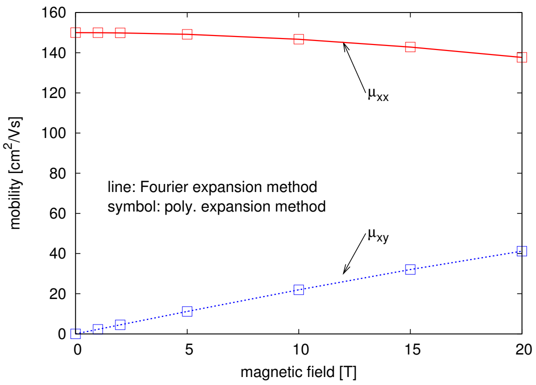

Figure 5: Mobilities for strong magnetic fields calculated by the Fourier and polynomial expansion method for an analytical spherical band.

MOSFETs," in *Proc. ESSDERC*, (Grenoble, France), pp. 561–564, 2005.

[3] A. T. Pham et al., "Physics-based modeling of hole inversion layer mobility in strained SiGe on insulator," *IEEE Trans. Electron Devices*, 2007.

[4] C. Jungemann et al., "A Linear Response Monte Carlo Algorithm for Inversion Layers and Magnetotransport," *Journal of Computational Electronics*, 2006.

[5] S. Takagi et al., "On the universality of inversion layer mobility in Si MOSFET's: Part I–Effects of substrate impurity concentration," *IEEE Trans. Electron Devices*, vol. 41, pp. 2357–2362, 1994.

[6] H. Irie et al., "In-Plane Mobility Anisotropy and Universality Under Uni-axial Strains in n- and p-MOS Inversion Layers on (100), (110), and (111) Si," in *IEDM Tech. Dig.*, 2004.