A Linear Response Monte Carlo Algorithm for Inversion Layers and Magnetotransport

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INTRODUCTION

Simulation of deca nanometer MOSFETs requires at least Monte Carlo (MC) models. Since no first principles scattering model for inversion layers exists, semiempirical models have to be used. Parameters of these models are determined by matching low-field measurements. Such simulations are extremely CPU intensive. We present a new linear response MC algorithm for electrons and holes in inversion layers and under the influence of an arbitrary magnetic field, which works even in the case of full band structures.

THEORY

The Boltzmann equation is linearized around equilibrium with respect to the driving electric field. In the case of an inversion layer this is the electric field in channel direction. Due to the symmetry of the problem the response of even expected values of the distribution function is quadratic in the driving field, and the first order response of the particle temperature or density and therewith of the electrostatic potential vanishes. Thus, a "frozen" electric field can be used at equilibrium. The linear response term in the Boltzmann equation is treated as a particle source, where only the positive part is considered due to symmetry at equilibrium. The approach is equivalent to a fluctuation dissipation theorem, where the integral over the conditional velocity is evaluated by an MC method.

RESULTS

All simulations are based on full band structures calculated by the nonlocal empirical pseudo potential method [1]. In Figs. 1,2 longitudinal (μ_{yy}) and transverse (μ_{zy}) hole mobilities are shown for strained and relaxed bulk Si as a function of the magnetic field, which is in one case applied parallel to the growth direction along the x-axis and in the other parallel to the driving field in y-direction. In the strained case the nonquadratic dependence of the mobility on the magnetic field is clearly visible. Moreover, the second order magnetotransport coefficient ($\alpha_{yy}^{x} = \sqrt{-1/\mu_{yy}\partial^2\mu_{yy}/\partial B_x^2|_{B_x=0}}$) is about twice the drift mobility. Thus the simple approximation of equating α and the drift mobility fails for holes. In strained Si for parallel electric and magnetic fields the longitudinal magnetotransport effect almost completely vanishes due to the less warped band structure. CPU times are about 30 CPU seconds per bias point, where the longitudinal mobility is accurate within 0.3%. In Figs. 3,4 effective hole mobilities for inversion layers are shown. The parameters of the surface scattering model were determined by matching experimental data. The CPU time per bias point is about 1 CPU minute for a stochastic error of 1%. Without the CPU efficient MC algorithm determination of the model parameters would have not been possible, because the CPU time would have been at least three orders of magnitude larger.

CONCLUSION

We have presented a novel linear response MC algorithm, which is many orders of magnitude faster than the conventional one, and works in the case of magnetotransport and inversion layers.

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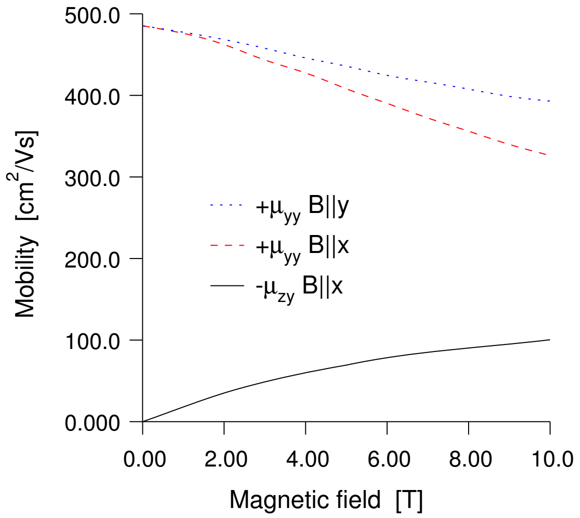

Fig. 1. Longitudinal and transverse mobilities for holes in undoped relaxed Si at room temperature for magnetic fields in x and y direction.

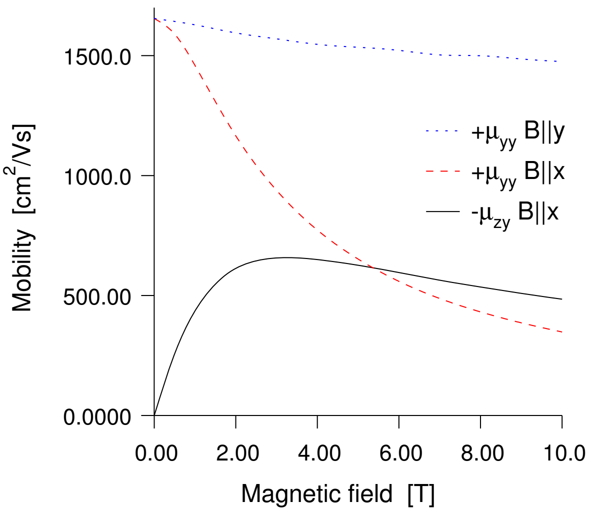

Fig. 2. Longitudinal and transverse mobilities for holes in undoped strained Si on $Si_{0.7}Ge_{0.3}$ at room temperature for magnetic fields in x and y direction.

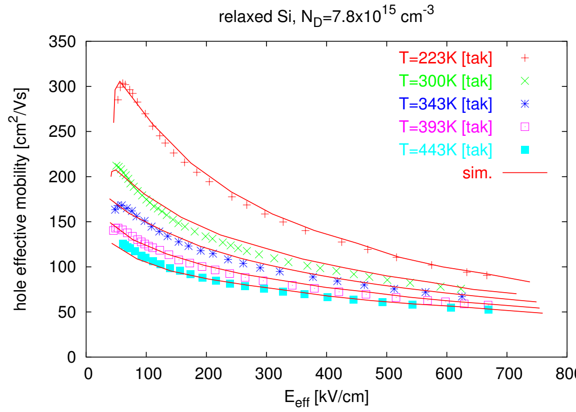

Fig. 3. Simulated effective hole mobility for a silicon inversion layer and measurements [2].

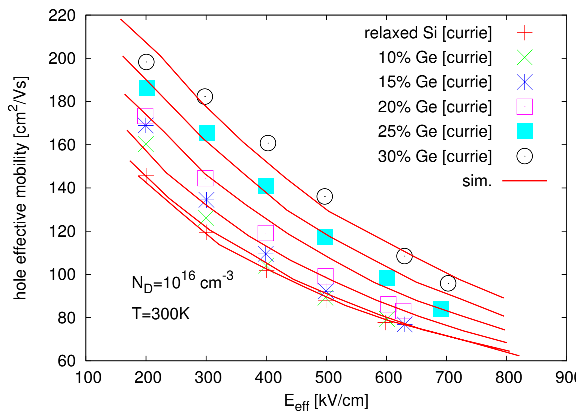

Fig. 4. Simulated effective hole mobility for a strained silicon inversion layer on relaxed $Si_{1-y}Ge_y$ and measurements [3].