Modeling Hole Surface- and Bulk-Mobility in the Frame of a Spherical-Harmonics Solution of the BTE

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Abstract

In a spherical-harmonics expansion formulation of the semi-classical Boltzmann transport equation (BTE) the influence of surface-scattering mechanisms on mobility are investigated, accounting for both global and local scattering mechanisms, with reference to holes in silicon. The analysis successfully reproduces the experimental data.

1. Introduction

The Spherical-Harmonics Expansion (SHE) method is applied to the Boltzmann Transport Equation (BTE), including the main scattering mechanisms and a numerical energy-band structure, in order to obtain a semiconductor-device solver able to give an accurate description of the energy distribution function and microscopic scattering rates. Thus, a computationally-effective solution of the BTE can be achieved, accounting for the main physical aspects. Preliminary tests have been carried out on the accuracy of the distribution function in the homogeneous case by means of an exhaustive investigation of the electron- and hole-mobility models, including the doping and temperature dependence [1, 2]. In [3], the introduction of the surface-scattering mechanisms into the SHE model has been presented, with respect to the electrons in the conduction band. In this work, following the above mentioned works, we present new results obtained in the investigation of the main transport properties in the frame of the SHE approach, specifically applied to holes. To this purpose, the analysis of the majority- and minority-hole mobilities is carried out with respect to the dependence on doping concentration, and the impurity-scattering mechanism is extended to give a complete description in both the bulk and channel structures. As for the surface-induced scattering mechanisms, namely, surface-roughness, surface acoustic phonons and charge centers at the interface, we use a two-dimensional description of the carriers (i.e., holes) in the region where a quantum confinement occurs, and compute the corresponding scattering terms. We calculate the inversion-layer hole mobility in a Si MOSFET, consistently with [4], and compare the inversion-layer mobility vs. effective electric field with experimental data. Results show that the SHE code successfully reproduces the universal behavior of the effective hole mobility.

2. Physical model

The general features of the spherical-harmonics solution of the BTE are illustrated in [5] and in the references therein. The method incorporates the main scattering mechanisms in silicon (acoustic phonons, optical phonons, ionized impurities, impact ionization). In addition, it accounts for the full band structure of the semiconductor, which is included through the density of states $g(E)$ and the group velocity $u_g(E)$ defined in the energy space; the latter are obtained directly from the corresponding functions in the momentum space (taken from the full-band system of [6]) by integrating over the angles. The energy range considered here allows for the description of the carrier dynamics up to 5 eV. As for the two-dimensional scattering mechanisms, they have been included using a consistent approach [3], that describes carriers in the region where a quantum confinement occurs. In this work, the effective width of the inversion layer, where the surface-scattering events take place, is calculated with the expression given in [7]. The collision mechanisms which are considered at the Si-SiO_2 interface are: surface roughness, scattering with ionized impurities trapped at the interface and surface phonons.

3. Homogeneous transport

The scattering mechanisms considered for the bulk structure are acoustical- and optical-phonon scattering, and ionized-impurity scattering. A number of extensions have been introduced in the ionized-impurity collision term. The effects of the Born approximation of order higher than one for incoherent collisions with a single impurity and for coherent collisions with impurity-pairs are accounted for. Impurity clustering, relevant for high doping concentrations, is implemented, following the work of [8]. At high doping densities the carrier scatters with a cluster of Z ions, where the clustering function Z depends on the impurity concentration. The effect of incomplete ionization of dopant has been introduced to account for the behavior of carrier mobility at high impurity concentrations and low temperatures, along with the description of the equilibrium carrier concentration in terms of Fermi statistics. Finally, different scattering terms are carried out for majority- and minority-mobility calculations. In particular, minority-hole mobility is found to be about a factor 2 higher than the majority-hole mobility for identical doping levels. In Fig.1, the majority- and minority-hole mobilities are reported as functions of impurity concentration.

4. Surface-scattering effects

As for the surface-induced scattering mechanisms, they must be treated differently from those relative to a bulk system because of localization. To take them into account we use a two-dimensional description of the carriers in the region where a quantum confinement occurs, and compute the corresponding scattering terms. The three scattering mechanisms which have been considered in presence of an interface are: i) Surface roughness, described in terms of its height Δ and correlation length L according to [7]; ii) Surface phonons, described as elastic phonons whose effect decays exponentially away from the interface; iii) Scattering with N_f charged centers located near the Si-SiO_2 interface, which originate from disorders and defects of the crystalline structure. In the adopted formulation of the surface-roughness scattering [3], the average of the electric field in the inversion layer is given by $E_{av} = (Q_{sc} + Q_b)/2\varepsilon_{si}$, where Q_{sc} is the space charge, Q_b is the depletion-region charge, and ε_{si} the dielectric constant of Si. The above definition of E_{av} represents also the effective electric field

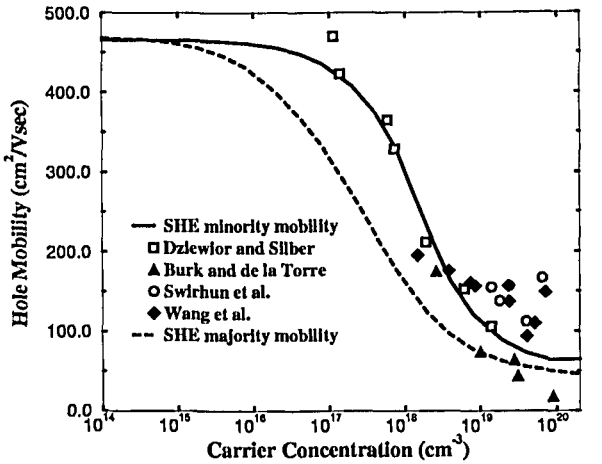

Figure 1: Calculations and experimental values of minority hole mobility [9]. The solid line is obtained with the SHE code calculations for a n-type Si bulk, the dashed line is the majority hole mobility.

to be used in the universal-mobility law for electrons. On the contrary, the effective field to be used for holes is $E_{\text{eff}} = (Q_b + 11/32Q_i)/\varepsilon_{si}$, where Q_i is the inversion-layer charge. Another difference in the modeling of hole mobility is that, in the definition of the surface-phonon scattering term, the two-dimensional density of Si is obtained multiplying the density ρ by the thickness of the inversion layer, given in [7].

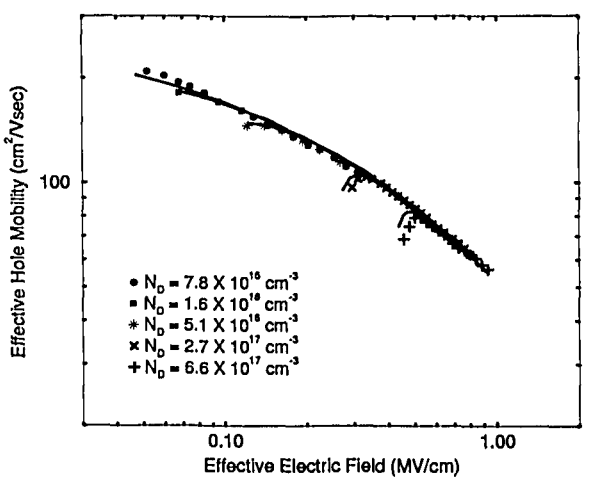

Figure 2: Hole mobility in inversion layer at 300 K versus effective field. The solid lines are obtained with the SHE code calculations.

5. Results

To check the soundness of the scattering models, the investigation of the majority hole mobility as a function of impurity concentration and temperature has been carried out first in the low-field regime for a bulk structure. At substrate doping concentrations greater than 10^{16} cm^{-3}, the large difference of majority- and minority-hole mobility is accounted for by means of a modification in the impurity scattering term, that gives the results shown in Fig.1. To investigate the universal behavior of the inversion-layer mobility, a number of simulations have been performed on a long channel p-MOS transistor with different substrate concentrations [4]. The device has 200 μm gate length, 25 nm oxide-thickness and substrate doping ranging from 7.8 10^{15} to 5.1 10^{16} cm^{-3}. The mobility behavior has been analyzed with a longitudinal field of 2.5 V cm^{-1} for different values of the transverse field. The result, shown in Fig. 2, was obtained by assuming typical values for the scattering parameters, namely Δ =2.5 Å, L =15 Å, and $N_I = 10^8$ cm^{-2}.

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