Hall Mobility Maps for 4H-Silicon Carbide by Monte Carlo Simulations

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Abstract. The Monte Carlo Single Particle approach was used to analyze electron transport in 4H-SiC taking into account the influence of the magnetic field. Within the numerical approach it was possible to evaluate electron Hall mobility and the Hall factor for the wide range of donor concentrations and temperatures varying from 300 K up to 700 K.

1. Motivation
The Silicon Carbide (SiC) is the wide band gap semiconductor which technology is under continuous development. Due to properties of its hexagonal politypes (6H-SiC, 4H-SiC) the SiC is dedicated to high temperature-, high frequency- and power-electronics. During last years, mostly due to technological problems eq. degradation of transport parameters during SiC processing a lot of research groups directed their attention to GaN. However it appeared that due to lack of good quality GaN monocrystals some attention was turned back to SiC in the field of high voltage devices [1]. Thus it seems that currently SiC is the only material appropriate for high power electronics [1]. Still there is lack of complete database of macroscopic parameters like mobility where the dependence on a wide range of environmental parameters (temperature, dopant concentration, crystallographic orientation) would be included. Measurements of SiC drift mobility $\mu_D$ [2] required special geometries and were done for very limited cases. More popular measurements of mobility utilize Van Der Pauw approach [3], but then the Hall mobility $\mu_H$ is measured which is different to the drift mobility. To find missing values of macroscopic transport parameters the computational physics can be utilized. The method selected should be based on basic physical phenomena valid for wide range of external conditions but still it has to computationally effective. These requirements are fulfilled by the Single Particle Monte Carlo Method (SPMC) [4] used widely to investigate charge transport in semiconductors [5]. With SPMC applied to SiC with magnetic field included one can calculate both $\mu_D$, $\mu_H$ and its ratio, the Hall factor $r_H$, for wide range of doping concentration and temperatures thus it also allows for recalculation of each type of mobility when the other is obtained by mean of other approach eq. from measurements. Within this paper we would like to present results for electron mobility calculation since electron unipolar SiC high power devices are being currently developed due to nearly one order higher mobility of electrons compared to holes [6,12].

2. Model
The Single Particle Monte Carlo approach was used to analyze the electron transport in 4H-SiC. The models utilized are described in [9]. Following models were used:
- single valley analytical non-parabolic ellipsoidal band-structure
- analytical description of the following scatterings: ionized impurities, acoustic phonon, zero order non-polar optical phonon, first order non-polar optical phonon, polar optical phonon, impact ionization
- the magnetic and electric field were simply taken into account using the following equations

\[
\Delta k_E = -\frac{eE}{\hbar} \tau_f
\]

\[
\Delta k_B = -\frac{v \times B}{\hbar} \tau_f
\]

where \(\Delta k_{(E,B)}\) – wave vector change due to presence of electric \(E\) and magnetic \(B\) field, \(\tau_f\) – free flight time, \(\hbar\) - reduced Planck constant, \(e\) – electron charge.

The use of analytical band-structure is justified since the mobilities and Hall factor should be evaluated for low range of energies to obtain correct value of \(\tau_H\) which is calculated for constant value of \(\mu_H\) and \(\mu_D\). The use of Monte Carlo method was previously considered inadequate [10] for evaluation of \(\mu_H\) due to weak effect of magnetic field in comparison to the thermal noise. However we found that the Monte Carlo method can be used to calculate the effect of magnetic field for the temperature range up to 700 K and for wide range of donors concentration. The magnetic field \(B\) we used during simulation was equal up to 2 T which is a value used in Van Der Pauw method measurements systems [7]. The electric field \(E\) must be lower than \(1E+6\) V/m to provide linear dependence of drift velocity on \(E\). However one should keep \(E\) high enough to reduce the influence of the thermal noise.

3. Results
With the Monte Carlo tool proposed it was possible to obtain 4H-SiC electron Hall mobilities for different orientation of the crystal, figure 1. The average anisotropy ratio between Hall mobilities for different crystal orientation is found to be 0.7, which is close to 0.8 reported in literature for the drift mobility [11].

![Figure 1. 4H-SiC electron Hall mobility as a function of temperature for different crystal orientation.](image)

One can also use the method to obtain the whole map of the 4H-SiC electron Hall mobilities as a function of temperature and dopant concentration. Such map is presented in figure 2. Similar maps could be obtained from analytical models eq. the Caughey-Thomas (C-T) model [8,11] which also takes into account influence of doping concentration and temperature. Comparison with this model
having parameters taken from [6] is depicted in figure 3. For the sake of clarity only contours of such maps are presented. The shape of the mobility maps for both methods is the same. However the values obtained from Caughey-Thomas model are higher in the range of lower temperatures and dopant concentrations. This could be explained by the fact that the Caughey-Thomas model reflects empirical dependence and is based on measurements of limited number of SiC crystal samples. The Caughey-Thomas (or any) empirical model reflects carrier transport in certain set of samples or some average of different measurements done by different groups and do not contain direct information about the physics inside. The proposed Monte Carlo method includes basic physics and is also depended on certain set of parameters. However the advantage of Monte Carlo simulations is that it is based on physical models and can be extended to catch other phenomena of carrier transport in SiC, eg. crystal defects.

**Figure 2.** Electron Hall mobility map perpendicular to c-axis.

**Figure 3.** Electron Hall mobility map perpendicular to c-axis compared with Caughey-Thomas model.
Measurement results of the Hall mobilities available in the literature [12,13] are also shown in figure 4.

![Figure 4. 2D cross-sections of the Hall mobility map from figure 2 compared with measurement results taken from literature a) [12], b) [13].](image)

Comparison presented in figure 4 shows that the calculated Hall mobility are in the range of measured values [12,13]. No perfect matching can be caused by different quality of SiC samples. The SiC crystal quality is continuously improving but it may be still defected during fabrication processes thus comparing simulation data with referenced measurements is difficult. Taking into account crystal defects in simulations is planned in future.

The calculated Hall factor is depicted in figure 5. Having knowledge about this parameter one can recalculate $\mu_H$ obtained from measurements to receive proper value of $\mu_D$.

Comparison with data available in literature [14,15] (figure 6) shows that obtained $r_H$ agrees with values obtained by other methods. Unfortunately, to the best knowledge of the author, there is no reference data for temperatures higher than 400 K.
4. Summary
By mean of the Monte Carlo method it is possible to evaluate the Hall electron mobility $\mu_H$ and Hall factor $r_H$ for 4H-SiC. Previously the Monte Carlo method was used to evaluate drift mobilities which could not be directly compared with large set of measurements since most of the measurements were done using Van Der Pauw method where the $\mu_H$ is obtained. With $\mu_H$ obtained from Monte Carlo one can evaluate maps of parameters that can be used in other CAD tools. Moreover direct access to measured and simulated $\mu_H$ allows for scattering model corrections which makes possible the creation of unique mobility maps (as function of eq. doping, temperature) for specific 4H SiC wafers.

5. References
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