Monte Carlo simulations of hole transport in 4H-SiC using DOS calculations

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Abstract. In this article we show results of 4H-SiC Monte Carlo simulation of hole transport based on numerically calculated density of states. As a result of these simulations the hole mobility for low electric field is obtained. To properly include scattering on ionized acceptor dopants the Brooks-Herring and Conwell-Weisskopf models are used.

1. Introduction
To simulate carrier transport for the present electronics we need a simulation tools which are able to combine atomic scale simulation and continue domain of semiconductor devices. In this article we focused on 4H-SiC wide band-gap semiconductor which is used for power devices [1]. The Monte Carlo method [2] takes scattering events and band structure model to investigate the hole transport. Then the macroscopic mobility is obtained from averaging the drift velocity with respect to external electric field. Approach described in [2] takes into account analytical formulas for energy band structure and density of states. In [3] it was proposed to use simple equations of scattering rates and combine these formulas with numerically calculated DOS. Results for electron transport simulation have been reported by the authors in [4, 5]

2. Materials and methods
2.1. Monte Carlo method
One of the most important properties quantities utilized by Ensemble Monte Carlo method are scattering phenomena. Within this work following scatterings are considered:

• Acoustic phonon scattering
\[ \Gamma_{ac}(E) = \frac{\pi \Xi_d^2 k_B T}{\hbar c_L} \text{DOS}(E) \]

where \( T \) is the temperature, \( c_L = \nu_s^2 \rho \) with \( \nu_s \) - the sound speed in 4H-SiC, \( \rho \) the mass density, \( \Xi_d \) - acoustic phonon deformation potential, \( E \) - hole energy

• Impurity scattering. To simulate the whole range of acceptor dopant density the following models are used:
Brooks-Herring (BH) model. It assumes that presence of the ionized impurity are extend to infinity. It is valid for small and medium dopant densities

\[
\Gamma_{BH}(E) = \frac{\pi N_I Z^2 e^4}{\epsilon_s^2 h 4 \pi^2 h^3 q_D^2 \left(4 k^2 + q_D^2\right)} DOS(E)
\]

where \( q_D = \sqrt{\frac{\epsilon S N_I}{\epsilon_s k_B T}} = \frac{1}{\lambda_D} \), \( N_I \) is the density of ionized impurities, \( \epsilon_S \) is the 4H-SiC dielectric permittivity, \( Z = 1 \), \( e \) - elementary charge, \( k \) - the wave vector, \( \lambda_D \) - Debye length.

Conwell-Weisskopf (CW) model. It assumes that the impurity affects electrostatic potential to the half of average distance to the nearest impurity. This model should be used for high dopant densities [6].

\[
\Gamma_{CW}(E) = \frac{2 (\hbar \pi)^3 N_I \left(\frac{3}{4 \pi N_I}\right)^2}{m_d^2 (1 + \alpha E)} DOS(E)
\]

where \( m_d \) is the effective density of states, \( \alpha \) - nonparabolicity parameter of the energy band model.

To switch between models we are using following condition:

\[
\sqrt{\frac{E (1 + \alpha E)}{4 \pi^2 h^3}} < b_{\text{max}}, \text{where } b_{\text{max}} = \sqrt{\frac{3}{4 \pi N_I}}
\]

Polar optical phonon scattering [3] for absorption and emission

\[
\Gamma_{\text{op,pol}}^{ab}(E) = \frac{\hbar \omega_{op}}{2 h \lambda^2 \pi \epsilon_p} \ln \left(\sqrt{\frac{E}{\hbar \omega_{op}}} + \sqrt{1 + \frac{E}{\hbar \omega_{op}}}\right) N \left(\frac{\hbar \omega_{op}}{C_{\text{pol}}}\right) DOS(E + \hbar \omega_{op})
\]

\[
\Gamma_{\text{op,pol}}^{em}(E) = \frac{\hbar \omega_{op}}{2 h \lambda^2 \pi \epsilon_p} \ln \left(\sqrt{\frac{E}{\hbar \omega_{op}}} - 1 + \sqrt{1 + \frac{E}{\hbar \omega_{op}}}\right) N \left(\frac{\hbar \omega_{op}}{C_{\text{pol}}}\right) DOS(E - \hbar \omega_{op})
\]

where \( \hbar \omega_{op} \) is the polar optical phonon energy, \( N \left(\hbar \omega_{op}\right) \) is the phonon number calculated by Bose–Einstein distribution, and

\[
\frac{1}{\epsilon_p} = \frac{1}{\epsilon_{\text{inf}}} - \frac{1}{\epsilon_s}
\]

with \( \epsilon_s \) and \( \epsilon_{\text{inf}} \) being a low and high frequency dielectric constants respectively.

Non-polar optical phonon scattering for absorption and emission

\[
\Gamma_{\text{op, pol}}^{ab}(E) = Z_H \frac{\pi D_H^2}{2 \omega_{op}} \left(N \left(\hbar \omega_{H}\right) + \frac{1}{2} \right) DOS((E) \pm \hbar \omega_{H})
\]

where \( \hbar \omega_{H} \) is the non polar optical phonon energy, \( Z_H = 3 \) for 4H-SiC \( N \left(\hbar \omega_{H}\right) \) - phonon number calculated by Bose–Einstein distribution and \( D_H \) - polar optical deformation potential.

Comparison of scattering rates for concentration \( N_I = 10^{18} \text{cm}^{-3} \) is presented in figure 1. The parameter used to calculate the scattering rates are shown in the table 1.
Figure 1. Scattering rates for impurity concentration $N_D = 10^{18} \text{cm}^{-3}$.

Table 1. Parameters used for scattering rates calculation.

| Symbol and unit | Parameter                                      | Value                  |
|-----------------|------------------------------------------------|------------------------|
| $\nu_s \left[ \frac{m}{s} \right]$ | sound speed in 4H-SiC | 13730 [7] |
| $\rho \left[ \frac{kg}{m^3} \right]$ | mass density | 3211 [7] |
| $\Xi_d \left[ eV \right]$ | acoustic phonon deformation potential | 9.0 [7] |
| $\epsilon_S \left[ - \right]$ | low frequency dielectric permittivity | 9.67 [7] |
| $\epsilon_{inf} \left[ - \right]$ | high frequency dielectric permittivity | 6.5 [7] |
| $\alpha \left[ \frac{1}{eV} \right]$ | nonparabolicity parameter of the energy band model | 0.323 [9] |
| $\hbar \omega_{op} \left[ eV \right]$ | polar optical phonon energy | $120 \cdot 10^{-3}$ [7] |
| $\hbar \omega_{H} \left[ eV \right]$ | non polar optical phonon energy | $85.4 \cdot 10^{-3}$ [10] |
| $D_H \left[ \frac{eV}{m} \right]$ | polar optical deformation potential | $2.8 \cdot 10^{11}$ [7] |

2.2. Calculation of DOS

The DOS for 4H-SiC has been calculated by the means of MedeA VASP software [11, 12]. As result of ab initio calculation one can get an effective DOS function. We show that it is possible to consider single hole particle model with the effective mass assigned. By the means of non-parabolic analytic dispersion relation (8) and Monte Carlo method it is possible to calculate proper values of hole mobility.

$$DOS(E)_{light, heavy} = 2 \left( \frac{2m^*_d \text{light(heavy)}}{4\pi^2\hbar^3} \right)^{3/2} \sqrt{E(1 + \alpha E)} \frac{\sqrt{E(1 + \alpha E)}}{(1 + 2\alpha E)}$$

(8)
where \( m_{d \text{ light(heavy)}}^* = \left( m_{l \text{ light(heavy)}} m_{l \text{ light(heavy)}} m_{l \text{ light(heavy)}} \right)^{1/3}, \alpha = 0.323, \]
\[
[m_{l \text{ light}}; m_{l \text{ light}}] = [1.64; 0.34] \text{ and } [m_{l \text{ heavy}}; m_{l \text{ heavy}}] = [1.64; 3.04] \text{ of electron mass } m_0 \text{ [13].}
\]
For the effective DOS which is the sum of DOSs of light and heavy holes one can calculate an effective mass as:
\[
m_t = \left( m_{t \text{ heavy}}^{3/2} + m_{t \text{ light}}^{3/2} \right)^{2/3}
\]
(9)

To compare the results obtained from ‘ab-initio’ DFT calculations the values from analytical formula (8) of DOS for light and heavy holes have also been plotted in figure 2.

**3. Results**

To calculate mobility by whole range of impurity concentration two models of ionized impurity scattering rates are used, i.e. the BH and CW models. These Ensemble MC simulations have been done for 1000 quasiparticles at room temperature with the final time of 0.1 ps and the time step \(10^{-14}\) s. The electric field was uniform \( E = 250 \text{ kV/m}\). Results of mobility simulation compared with measurement data are shown in figure 3.
4. Conclusions
 Within this paper it was shown that by the appropriate use of BH and CW scattering models it is possible to obtain correct value of hole mobility for the entire range of acceptor dopant concentration. The routine proposed in this article can be used for any semiconductor including also crystals with defects. We have shown that by means of DFT simulations and Monte Carlo method it is possible to create link between world of atoms and continues domain of solid state electronics.

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