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Accurate Modeling of Lattice Site-Dependent Incomplete Ionization in α-SiC Devices Ayalew T.¹, Grasser T.¹, Kosina H.² and Selberherr S.²

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In contrast to narrow bandgap semiconductors such as silicon, common doping impurities in SiC have activation energies larger than the thermal energy k_BT even at room temperature. This causes the incomplete ionization of such impurities, which leads to a strong temperature and frequency dependence of the semiconductor junction differential admittance [1]. Inequivalent sites of α -SiC, C (or Si) sites, one with cubic (k) surrounding and the other with hexagonal (h) surrounding are expected to cause site-dependent impurity levels [2]. In that case the single effective level assumption of donor impurities, $\Delta E_{\rm D} = E_{\rm C} - E_{\rm D}$, commonly used in numerical simulation should be expanded to account for the site-dependent ionization energy of the α -SiC polytypes. Thus, for donor impurities, the electron carrier concentration determined from the neutrality condition of the Poisson equation (1) should be simplified to (2)

$$\operatorname{div}(\varepsilon \cdot \operatorname{grad} \psi) = \operatorname{q} \cdot (n - p + N_D^+ - N_A^-) \qquad (1) \qquad n = \sum_{i=1}^x N_{D \, h_i}^+ + \sum_{j=1}^y N_{D \, k_j}^+$$
 (2)

where x and y are the number of inequivalent hexagonal and cubic sites in α -SiC, respectively. 4H-SiC consists of x=y=1, 6H-SiC is composed of x=1 and y=2, and 15R-SiC has x=2 and y=3. The 4H-SiC possesses two impurity levels with ionization energies ΔE_{Dh} and ΔE_{Dk} for hexagonal and cubic donors, respectively. The degree of ionization ξ_{D} for this polytype will then have a form

$$\xi_{\mathrm{D}} = \frac{N_{\mathrm{D}}^{+} + N_{\mathrm{D}}^{+} + N_{\mathrm{D}}^{+}}{N_{\mathrm{D}}} = \left[2 + 2g_{\mathrm{D}} \frac{n}{N_{\mathrm{C}}} \cdot \exp\left(\frac{\Delta E_{\mathrm{Dh}}}{k_{\mathrm{B}} \cdot T_{\mathrm{L}}}\right) \right]^{-1} + \left[2 + 2g_{\mathrm{D}} \frac{n}{N_{\mathrm{C}}} \cdot \exp\left(\frac{\Delta E_{\mathrm{Dk}}}{k_{\mathrm{B}} \cdot T_{\mathrm{L}}}\right) \right]^{-1}$$
(3)

where $g_{\rm D}$ with a typical value of 2 is the degeneracy factors for the impurity levels of donors in α -SiC, $N_{\rm C}$ is the effective density of states in the conduction band, and $T_{\rm L}$ is the lattice temperature. Fig. 1 and Fig. 2 illustrate the carrier concentration ionization degree as a function of concentration and temperature for the site-dependent nitrogen (N) ionization energy of $\Delta E_{\rm Dh}$ =50 meV and $\Delta E_{\rm Dk}$ =90 meV [3], and the commonly used effective ionization energy value of $\Delta E_{\rm D}$ =70 meV. Here, for temperatures of only 100 K and $N_{\rm D}=10^{15}~{\rm cm}^{-3}$, 60% of N is ionized as a result of the site-dependent ionization energy, while 50% of N is ionized by using the effective ionization energy assumption in 4H-SiC. At room temperatures and a donor concentration of $N_{\rm D}=10^{19}~{\rm cm}^{-3}$, only 30% of N is ionized using site-dependent ionization energy, while 5% is ionized by using effective ionization energy. Therefore, numerical investigation results for α -SiC without using lattice site-dependent incomplete ionization are at least questionable.

The new model was implemented into the general-purpose device simulator Minimos-NT [4] and allows for quantitative simulation of devices based on different α -SiC polytypes. We simulate a UMOSFET fabricated from 4H-SiC with a drift region concentration of $1.5 \times 10^{16} {\rm cm}^{-3}$, a p-base region concentration of $1.0 \times 10^{17} {\rm cm}^{-3}$, and a source region concentration of $1.0 \times 10^{19} {\rm cm}^{-3}$. The simulation result of the carrier mobility using the site-dependent incomplete ionization model for a drain-to-source voltage of $V_{\rm DS}=5 {\rm V}$ and a gate-to-source voltage of $V_{\rm GS}=10 {\rm V}$ at room temperature is shown in Fig. 3. From the room temperature carrier concentration level mentioned above, one can see a considerable differences in the amount of current that a transistor can carry between the two ionization energy levels, as depicted in Fig. 4. As the temperature is increased well above 300 K, the resulting increase in carrier concentration with temperature reduces the differences. From the mobility data and the carrier concentration level mentioned above, the resistivity ρ in n-type α -SiC material can be calculated by $\rho_n = \left[{\rm q} \cdot \mu_n \cdot (N_{\rm D}^+ + N_{\rm D}^+ k) \right]^{-1}$. At high doping levels and increasing temperature, the increasing dopant ionization level overcompensates the decreasing mobility. The resistivity then decreases with increasing temperature, as can be seen in Figs. 5.

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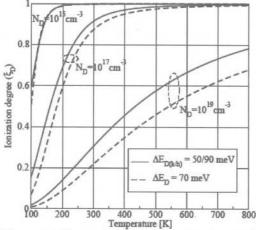


Figure 1: Comparison of Ionization degree of donors (N) using site-dependent and effective activation energy in 4H-SiC.

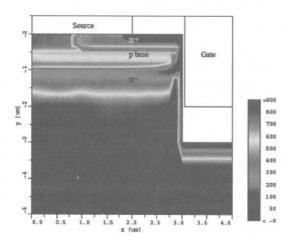


Figure 3: The carrier mobility in a 4H-SiC UMOSFET at 300 K applying the site-dependent ionization level model.

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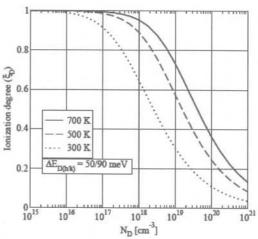


Figure 2: Ionization degree of donors (N) using the site-dependent activation energy in 4H-SiC.

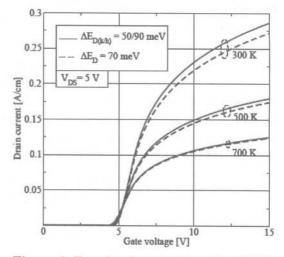


Figure 4: Transfer characteristics of a 4H-SiC UMOSFET using the site-dependent and effective activation energy.

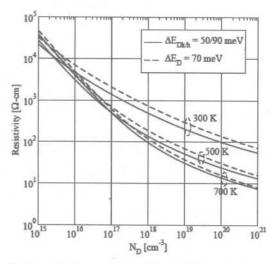


Figure 5: Comparison of resistivity of n-type 4H-SiC calculated from the dopingand temperature dependent mobility.