Modeling of Lattice Site-Dependent Incomplete Ionization in α-SiC Devices

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Abstract. In contrast to narrow bandgap semiconductors such as silicon, common doping elements in SiC have activation energies larger than the thermal energy $k_{\mathrm{B}}T$ even at room temperature. Inequivalent α-SiC sites, one with cubic (k) surrounding and the other with hexagonal (h) surrounding are expected to cause site-dependent impurity levels. Therefore, an appropriate incomplete ionization model which accounts for lattice site-dependent ionization level of impurities in α-SiC has been developed and implemented in the general-purpose device simulator MINIMOS-NT.

Introduction

At low temperatures the thermal energy within a semiconductor is not high enough to fully activate all of the donor and acceptor atoms. As a result the carrier concentration will not reach the concentration of dopant atoms [1]. SiC is different from narrow bandgap semiconductors, in that common dopants have activation energies larger than the thermal energy $k_{\mathrm{B}}T$ even at room temperature. This causes incomplete ionization of such dopants, which leads to a strong temperature and frequency dependence of the semiconductor junction differential admittance. Many dopants of SiC preferentially incorporates into either Si sites or C sites. N preferentially incorporates into the lattice sites which are normally occupied by C atoms. P and Al prefer the Si sites of SiC, whereas B may substitute on both sites [2]. Inequivalent sites of α-SiC, one with cubic surrounding and the other with hexagonal surrounding are expected to cause site-dependent impurity levels in n-type materials [3]. Therefore, numerical investigation results for α-SiC devices without using lattice site-dependent ionization level are questionable. In this work an appropriate incomplete ionization model which accounts for a polytype and lattice site-dependent ionization level of impurities in α-SiC has been developed and implemented into the general-purpose device simulator MINIMOS-NT [4].

Modeling

In addition to the substantial variation of ionization energies of donors with the SiC polytypes, inequivalent sites of α-SiC, either Si sites or C sites, one with cubic (k) and the other with hexagonal (h) surrounding are experimentally observed to cause site-dependent impurity levels [3]. In that case the single effective donor level assumption, $\Delta E_{\mathrm{D}} = E_{\mathrm{C}} - E_{\mathrm{D}}$, commonly used in numerical simulation should be expanded to account for the site-dependent ionization energy of the α-SiC polytypes

$$\Delta E_{\mathrm{Dh}} = E_{\mathrm{C}} - E_{\mathrm{Dh}}, \qquad \text{and} \qquad \Delta E_{\mathrm{Dk}} = E_{\mathrm{C}} - E_{\mathrm{Dk}} . \tag{1}$$

For donor impurities, the electron carrier concentration is determined from the charge neutrality condition of the Poisson equation, that is, the individual electron and hole current flowing across the junction are identically zero, and the Fermi level is constant. For this condition the right-hand side of the Poisson equation is simplified to

$$n + N_A^- = p + N_D^+, \qquad \text{with} \qquad N_D^+ = \sum_{i=1}^{x} N_{\text{Dh}_i}^+ + \sum_{j=1}^{y} N_{\text{Dk}_j}^+, \qquad (2)$$

where x and y are the number of inequivalent hexagonal and cubic sites in α-SiC, respectively. The 4H-SiC consists of $x = y = 1$ and 6H-SiC is composed of $x = 1$ and $y = 2$. The corresponding experimental values of the site-dependent ionization energy levels for Al, B, N, and P in 4H- and 6H-SiC are listed in Table 1 [5]. The concentration of ionized donor impurity atoms

	Al	B	N_h	N_k	P_h	P_k
4H-SiC	220 ± 20	330 ± 30	50 ± 5	90 ± 5	50 ± 5	90 ± 5
6H-SiC	220 ± 20	330 ± 30	80 ± 5	140 ± 5	80 ± 5	110 ± 10

Table 1: Site-dependent ionization energy (in meV) level for Al, B, N, and P in α-SiC.

is given by a steady-state Gibbs distribution

$$N_D^+ = \frac{N_D}{1 + g_D \dfrac{n}{n_1}}, \qquad \text{with} \qquad n_1 = N_C \cdot \exp\left(-\frac{\Delta E_{\text{Dh,k}}}{k_B T_L}\right), \qquad (3)$$

where N_D is the substitutional (active) dopant concentration for a donor, n is the free electron concentration, g_D with typical value of 2 is the degeneracy factor for the impurity level of donors in α-SiC, N_C is the effective density of states in the conduction band, and T_L is the lattice temperature.

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 be of the form

$$\xi_D = \frac{N_{Dh}^+ + N_{Dk}^+}{N_D} = \frac{1}{2 + 2g_D \dfrac{n}{N_C} \exp\left(\dfrac{\Delta E_{\text{Dh}}}{k_B T_L}\right)} + \frac{1}{2 + 2g_D \dfrac{n}{N_C} \exp\left(\dfrac{\Delta E_{\text{Dk}}}{k_B T_L}\right)}, \qquad (4)$$

$$\xi_D = \frac{-1 + \sqrt{1 + 2g_D \dfrac{N_D}{N_C} \exp\left(\dfrac{\Delta E_{\text{Dh}}}{k_B T_L}\right)}}{2g_D \dfrac{N_D}{N_C} \exp\left(\dfrac{\Delta E_{\text{Dh}}}{k_B T_L}\right)} + \frac{-1 + \sqrt{1 + 2g_D \dfrac{N_D}{N_C} \exp\left(\dfrac{\Delta E_{\text{Dk}}}{k_B T_L}\right)}}{2g_D \dfrac{N_D}{N_C} \exp\left(\dfrac{\Delta E_{\text{Dk}}}{k_B T_L}\right)}. \qquad (5)$$

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 $\Delta E_{\text{Dh}} = 50\,\text{meV}$ and $\Delta E_{\text{Dk}} = 90\,\text{meV}$, and the commonly used effective ionization energy value of $\Delta E_D = 70\,\text{meV}$. Here, for temperatures of only 100 K and $N_D = 10^{15}\,\text{cm}^{-3}$, 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 $N_D = 10^{19}\,\text{cm}^{-3}$, only 30% of N is ionized using a site-dependent ionization energy, while 5% is ionized by using effective ionization energy.

Application

The new model was implemented into the general-purpose device simulator MINIMOS-NT and allows for quantitative simulation of devices based on different α-SiC polytypes. We simulated a UMOSFET fabricated from 4H-SiC with a drift region doping concentration of $1.5 \times 10^{16} \text{cm}^{-3}$, a p-well region doping concentration of $1.0 \times 10^{17} \text{cm}^{-3}$, and a source region doping concentration of $1.0 \times 10^{19} \text{cm}^{-3}$. The carrier mobility using the site-dependent incomplete ionization model for a $V_{DS} = 5\,V$ and a $V_{GS} = 10\,V$ at $300\,K$ and $500\,K$ are shown in Fig. 3 and Fig. 4, respectively. 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. 5. 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

$$\rho_n = \frac{1}{q\mu_n(N_{D\,h}^+ + N_{D\,k}^+)}. \tag{6}$$

At high doping levels and increasing temperature, the increasing dopant ionization level over-compensates the decreasing mobility. The resistivity then decreases with increasing temperature, as can be seen in Fig. 6.

Conclusion

In addition to the substantial variation of ionization energies of donors with the SiC poly-types, inequivalent sites of α-SiC, one with cubic surrounding and the other with hexagonal surrounding are expected to cause site-dependent impurity levels. Therfore, an accurate model which accounts for polytype and lattice site-dependent ionization level of impurities in α-SiC has been developed and implemented in the general-purpose device simulator MINIMOS-NT. The model allows for quantitative simulation of α-SiC devices based on different polytypes and the presence of inequivalent sites. A UMOSFET fabricated from a 4H-SiC was simulated. The level of the carrier concentration and the resistivity in the device at different temperatures have been investigated.

Acknowledgment

References

[1] S. Selberherr, IEEE Trans.Electron Devices Vol. 36 (1989), p. 1464.

[2] T. Ayalew, Dissertation, *SiC Semiconductor Devices Technology, Modeling, and Simulation*, TU-Vienna, Austria (2004), http://www.iue.tuwien.ac.at/phd/ayalew/.

[3] M. Ikeda *et al.*, Physical Review B Vol. 22 (1980), p. 2842.

[4] *Minimos-NT, Device and Circuit Simulator, User's Guide*, Institute for Microelectronics, TU-Vienna, Austria (2002), http://www.iue.tuwien.ac.at/mmnt/.

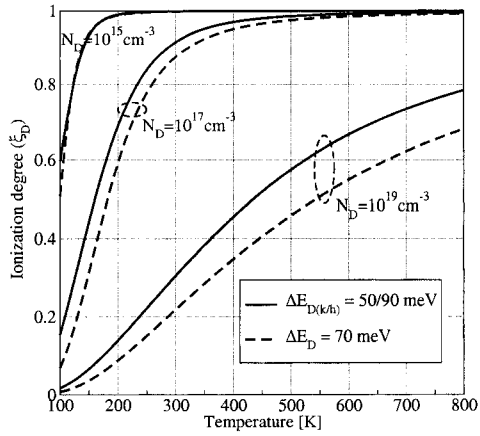[5] C. M. Zetterling, EMIS series, no. 2, INSPEC, IEE, UK (2002).

Fig. 1: Comparison of ionization degree of donors (N) assuming an effective and a site-dependent activation energy in 4H-SiC.
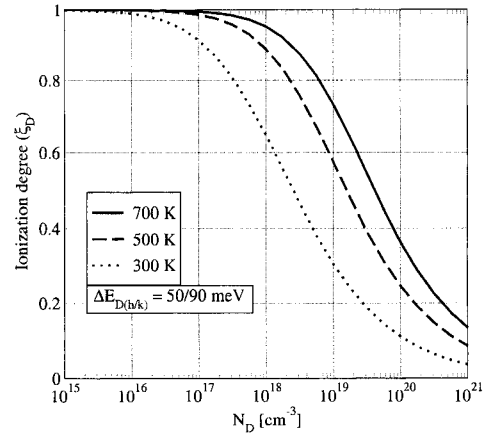

Fig. 2: Ionization degree of donors (N) assuming a site-dependent activation energy in 4H-SiC.
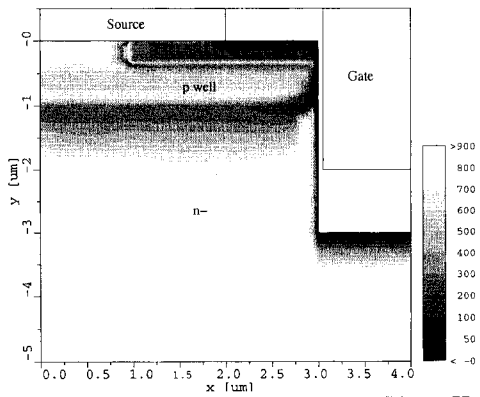

Fig. 3: The carrier mobility at 300K in 4H-SiC UMOSFET utilizing the lattice site dependent ionization level model.
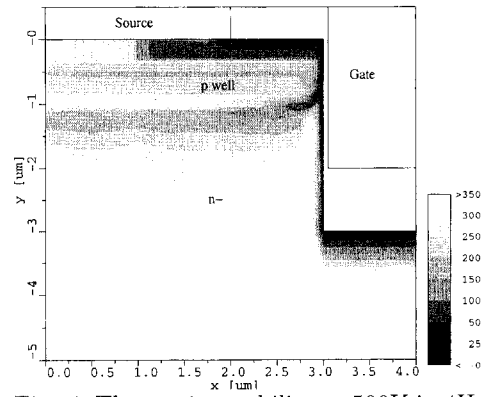

Fig. 4: The carrier mobility at 500K in 4H-SiC UMOSFET utilizing the lattice site dependent ionization level model.
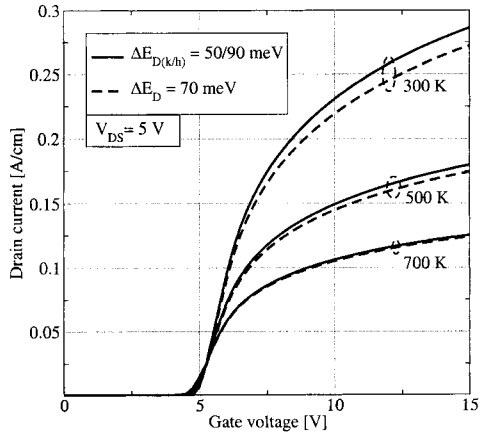

Fig. 5: Comparison of transfer characteristics of a 4H-SiC UMOSFET using an effective and a site-dependent activation energy.
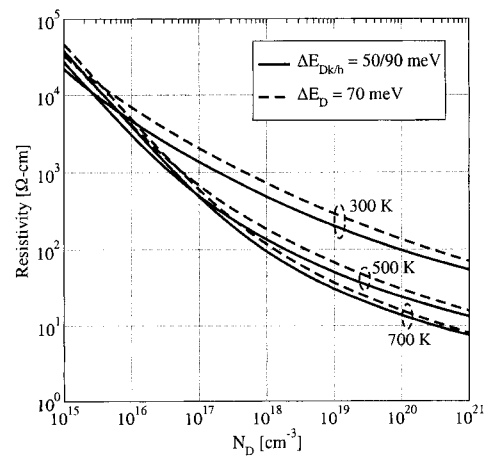

Fig. 6: Resistivity of n-type 4H-SiC calculated from the doping- and temperature dependent mobility.