Estonian Journal of Engineering, 2011, **17**, 2, 151–157 doi: 10.3176/eng.2011.2.05

Generalized analytical model for SiC polytypic heterojunctions

Toomas Rang[a], Indrek Tabun[a], Galina Rang[a] and Ants Koel[b]

[a] Thomas Johann Seebeck Department of Electronics, Tallinn University of Technology, Ehitajate tee 5, 19086 Tallinn, Estonia; trang@elin.ttu.ee
[b] ELION/Microlink Ltd, Lõõtsa 8, 11415 Tallinn, Estonia

Received 7 February 2011, in revised form 11 April 2011

Abstract. A new generalized analytical model has been developed for analysing SiC polytypic heterojunctions. The forward and reverse biasing situations have been investigated and two novel results have been detected. First, the activation energy plays a major role in the determination of the place of the so-called knee point. The smaller the activation energy, the lower value has the knee point. Similar behaviour has been observed also by the increase of the temperature. Second, the density of traps and their temperature behaviour limits the current approximately at 350 °C, which means that the increase of the reverse current and therefore the reverse biasing is not in correlation anymore.

Key words: semiconductors, heterostructures, silicon carbide, 3C and 4H-polytypes, U-I chatracteristics.

1. INTRODUCTION

SiC has been a suitable material for high temperature and high power applications due to its superior material as well as electrical properties over Si and GaAs and availability of different polytypes in SiC. Having the same chemical nature, SiC polytypes may significantly differ in their electrical parameters. In recent years, the interest in the fabrication and study of heteropolytype structures, based on SiC, has considerably increased. It has been shown that heterostructures between SiC polytypes may have better structural perfection than those constituted by semiconductors that differ in chemical nature. In [1], for example, the formation of two-dimensional electron gases (2DEGs) at polytypic (hexagonal/cubic) SiC heterojunctions (4H/3C SiC and 6H/3C SiC) is investigated by numerical self-consistent solutions of the Schrödinger and Poisson

equations. The combined effect of the polarization-induced bound charge and conduction-band offset between the hexagonal and cubic SiC polytypes results in the formation of 2DEGs with very high electron sheet concentration.

In recent years, new types of semiconductor heterostructures, consisting of only one material in different crystal structures, such as wurtzite/zinc-blende heterostructures (heteropolytypic structures) have been investigated. Such hetero-structures maintain a completely defect-free, lattice-matched, and coherent interface and the effects due to different chemical constituents can be avoided. In this field, SiC is the most promising candidate, because SiC crystallizes in more than two different stable structures. The preparation of heteropolytypic structures by only a change of the crystal structure during the growth is a great challenge. There are today two competitive possibilities to realize the polytypic hetero-junctions: well-defined molecular beam epitaxy (MBE) [2], and much more sophisticated wafer bonding technology (diffusion welding) [3]. On the basis of the MBE technology, the high current gain Darlington transistor, with a wide bandgap emitter having a very high current gain, obtained by implementing the concept of the heterojunction to increase the current gain of the Darlington transistor using 4H- SiC with a bandgap of 3.2 eV for the emitter and 3C-SiC with a bandgap of 2.2 eV for the base and the collector regions, has been introduced [4].

In this paper the generalized analytical model for polytypic heterojunctions is described. The model allows for the first time to analyse in a time consuming way the static characteristics of heterojunctions, taking into account the influence of the deep energy levels and other scattering processes inside and around the hetero-interface.

2. MODEL DESCRIPTION

Different SiC polytypes have widely varying physical properties. 3C-SiC has the highest electron mobility and saturation velocity because of reduced phonon scattering, resulting from higher symmetry. The band gaps differ widely among the polytypes, ranging from 2.3 eV for 3C-SiC to 3 eV for 6H SiC and to 3.3 eV for 2H-SiC. In general, the greater the wurtzite component, the larger the band gap. All these properties make the development of time consuming simulation models very difficult. We shall make an attempt to develop a new sophisticated analytical model, which includes almost all important physical parameters for the static analysis of the junctions, but remains still pretty simple from the point of view of calculations.

The generalized forward characteristic is based on the tunnel-recombination phenomenon and the forward current density J_f can be described as

$$J_f = J_{sat}\left(\exp\left(\frac{qV_f}{\eta k_b T}\right)-1\right), \quad \text{A/cm}^2, \tag{1}$$

where J_{sat} is the saturation current density, q is the electron charge, V_f is the forward voltage, η is the parametric constant describing the proportion of diffusion and recombination currents, k_b is the Boltzmann constant, and T is the absolute temperature.

The saturation current J_{sat} can be written as

$$J_{sat} = \frac{qs_j\sqrt{N_{cp}N_{cn}N_{vp}N_{vn}}}{N_{n0}}\exp\left(\frac{-E_A}{k_bT}\right), \tag{2}$$

where s_j is the recombination velocity, N_{cp} and N_{cn} are the state densities in conductive band (p- and n-regions respectively), N_{vp} and N_{vn} are the state densities in valence band (p- and n-regions, respectively), N_{n0} is the electron concentration outside the interface, and E_A is the activation energy.

The recombination velocity s_j, is calculated as

$$s_j = \sigma\nu_{th}N_r, \text{ cm/s}, \tag{3}$$

where σ is the cross-section area of the recombination centre, ν_{th} is the thermal velocity of charge carriers and N_r is the surface density of recombination centres.

The activation energy (internal potential) E_A is defined as

$$E_A = \frac{E_{gn}+E_{gp}}{2} - \frac{qV_0}{\eta_n} + \frac{q\Delta\psi}{\eta}, \tag{4}$$

where E_{gn} and E_{gp} are the band gaps (n- and p-regions, respectively), V_0 is the intrinsic contact potential and $\Delta\psi$ is the barrier contact potential. The temperature dependence of the activation energy is taken from [5]. The parametric constants η and η_n are calculated as

$$\eta = \frac{\eta_n}{\eta_n - 1}, \quad \eta_n = 1 + \frac{\varepsilon_p + N_d}{\varepsilon_n N_a},$$

where ε_n and ε_p are the dielectric permittivity of n- and p-regions, respectively.

The barrier contact potential $\Delta\psi$ and the intrinsic potential barrier V_0 can be expressed as

$$\Delta\psi = \Delta E_C + \frac{k_bT}{q}\ln\left[\frac{N_{cp}n_{in}}{n_{ip}N_{cn}}\right], \quad V_0 = \frac{k_bT}{q}\ln\left[\frac{N_aN_d}{n_{in}n_{ip}}\right], \tag{5}$$

where ΔE_C is the shift of the conductive band, n_{in} and n_{ip} are the intrinsic electron concentrations (for n- and p-regions, respectively), N_a and N_d are the acceptor and donor impurity concentrations, respectively.

The reverse current density J_r is defined as

$$J_r = \frac{-qN_t}{T_k}, \tag{6}$$

where N_t is the surface density of the traps and $T_k = T_\varepsilon + T_t$ is total time for the emission and tunneling processes.

The tunneling barrier is defined by the barrier height Ψ_B [6]:

$$\Phi_B = V_{bi} + V_n - \frac{k_b T}{q}, \tag{7}$$

where V_n is the potential between the conductive band up to the Fermi potential, and V_{bi} is the diffusion potential.

Using the described model, a MathCAD based algorithm has been developed and the simulations have been done.

3. RESULTS AND ANALYSIS

Under the investigation were the n-3C/n-4H and n-3C/n-6H heterojunctions. The impurity concentration in n-3C SiC was chosen $N_{D3C} = 6\times10^{16}$ cm^{-3}, and for the hexagonal SiC polytypes $N_{D4H} = N_{D6H} = 2\times10^{18}$ cm^{-3}. The band gaps of the polytypes depend on the temperature and impurity concentration. The typical value for the surface density of the traps is $N_t = 3.5\times10^{14}$ cm^{-2}. In [7] the shift of the band gap edges is defined as

$$\begin{aligned} \Delta E_C &= A_{nc}\left(\frac{N_D}{10^{18}}\right)^{1/3} + B_{nc}\left(\frac{N_D}{10^{18}}\right)^{1/2}, \\ \Delta E_V &= A_{nv}\left(\frac{N_D}{10^{18}}\right)^{1/4} + B_{nv}\left(\frac{N_D}{10^{18}}\right)^{1/2}, \end{aligned} \tag{8}$$

where the coefficients in Eq. (8) are given in Table 1.

The simulation results are shown in Fig. 1.

The simulations show that the knee point for heterojunction n-3C/n-6H arrives earlier compared to the heterojunction n-3C/n-4H. The explanation emerges directly from the value of the activation energy, which is smaller for the heterojunctions n-3C/n-6H. Figure 1a shows that similar behaviour of the knee

Table 1. Coefficients of Eq. (8) [7]

n-type	A_{nc}	B_{nc}	A_{nv}	B_{nv}
3C-SiC	–1.48E-03	–3.06E-03	1.75E-02	6.85E-03
4H-SiC	–1.50E-02	–2.93E-03	1.90E-02	8.74E-03
6H-SiC	–1.12E-02	–1.01E-03	2.11E-02	1.73E-03

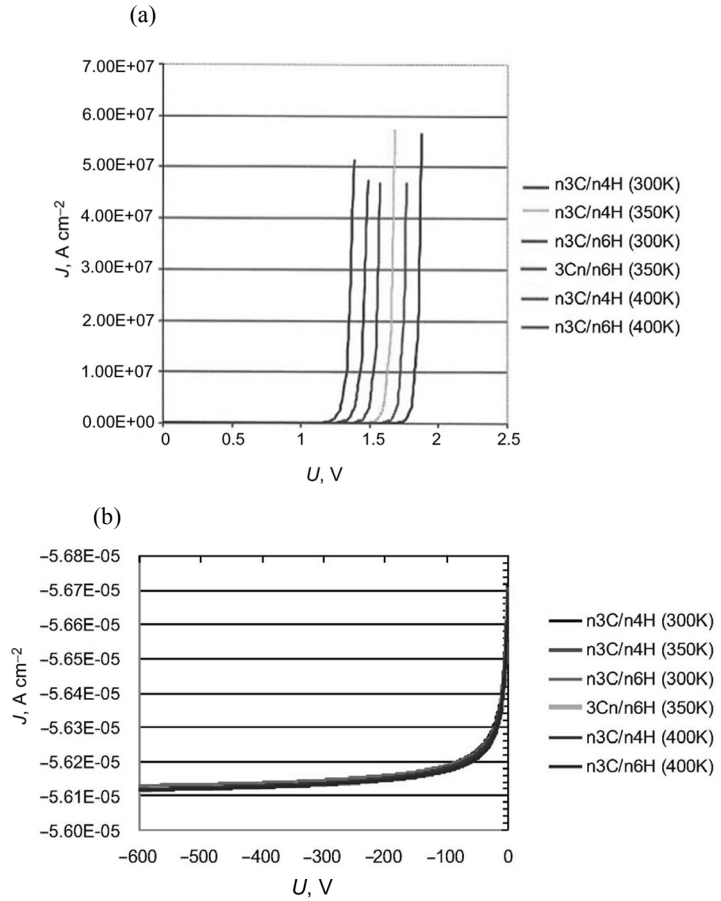

Fig. 1. Current density J vs applied voltage U at different temperatures: (a) forward characteristics ($J \equiv J_f$); (b) reverse characteristics ($J \equiv J_r$).

point can be observed by the increase of the temperature, because the activation energy decreases with the rise of the temperature. The reverse characteristics depend strongly on the density of the traps. Figure 1b indicates that for the reverse characteristics the influence of the temperature ceases at about 350°C. The reason is that the density of traps is almost saturated and no significant further increase of tunneling current takes place. The mechanism of the electron transport through the heterojunction is dual: first, the electrons move in 3C-SiC into the trap, which has the optimal level with the help of the tunneling mechanism and afterwards the thermal emission carries the electrons inside the hexagonal n-4H-SiC or n-6H-SiC into the conductive band. The simulations show that the distribution of the electrical field strength by the increase of reverse biasing moves towards the cubic polytype (n-3C-SiC) side of the heterojunction and therefore by the charge carriers transport the tunneling mechanism increases compared to thermal emission.

4. CONCLUSIONS

A generalized analytical model for the simulation of SiC polytypic heterojunctions has been developed and applied in the environment of MathCAD. With the model the following important novel results have been reached.

- The activation energy plays the major role in the determination of the location of the knee point. The smaller the activation energy the lower value has the knee point.
- The increase of the temperature causes a decrease of the activation energy and again the lower value of the knee point has been reached.
- The density of traps and their temperature behaviour limits the reverse current approximately at 350 °C, which means that the increase of the reverse current and therefore the reverse biasing are not in correlation anymore.

Our simulations lead also to the conclusion that some of the parameters of the analytical model and their behaviour need additional numerical analysis to ensure the validity of the model.

ACKNOWLEDGEMENT

The authors wish to thank the Estonian Ministry of Education and Research (the target oriented project SF0142737s06), the Estonian Science Foundation (grant 7183), and the Foundation Archimedes through the Centre of Excellence CEBE (TK05U01) for the support of the research.

REFERENCES

1. Polyakov, V. M. and Schwierz, F. Formation of two-dimensional electron gases in polytypic SiC heterostructures. *J. Appl. Phys.*, 2005, **98**, 023709-1–023709-6.
2. Fissel, A. Artificially layered heteropolytypic structures based on SiC polytypes: Molecular beam epitaxy, characterization and properties. *Phys. Reports*, 2003, **379**, 149–255.
3. Ivanov, P. A., Kostina, L. S., Potapov, A. S., Samsonova, T. P., Belyakova, E. I., Argunova, T. S. and Grekhov, I. V. Current–voltage characteristics of isotype SiC–SiC junctions fabricated by direct wafer bonding. *Fizika i Tekhnika Poluprovodnikov*, 2007, **41**, 941–944 (in Russian).
4. Luo, Y., Zhang, J., Alexandrov, P., Fursin, L. and Zhao, J. H. Fabrication and characterization of high current gain (β = 430) and high power (23 A-500 V) 4H-SiC hybrid Darlington bipolar transistor. *IEEE Trans. Electron Devices*, 2004, **51**, 2211–2216.
5. SiC band structure and carrier concentration. http://www.ioffe.ru/SVA/NSM/Semicond/SiC/bandstr.html
6. Seeger, K. *Semiconductor Physics*, 8th ed. Springer, Berlin, 2002.
7. Lindefelt, U. A model for doping-induced band-gap narrowing in 3C-, 4H-, and 6H-SiC. *Mater. Sci. Eng. B*, 1999, **61–62**, 225–228.

Üldistatud analüütiline mudel SiC-polütüüpsetele heterosiiretele

Toomas Rang, Indrek Tabun, Galina Rang ja Ants Koel

On välja töötatud üldistatud matemaatiline mudel SiC-polütüüpsete heterosiirete analüüsimiseks. On uuritud heterosiirete päri- ja vastupinge olukordi. Simulatsioonide tulemusena jõuti kahele olulisele tulemusele. Esiteks täheldati, et aktivatsioonienergia mõjutab oluliselt pärikarakteristiku murdepunkti selliselt, et väiksem aktivatsioonienergia nihutab murdepunkti väiksemate pingete väärtuste poole. Samasugust käitumist täheldati ka temperatuuri kasvades. Teiseks, lõksude tihedus ja nende temperatuurisõltuvus limiteerib vastuvoolu muutust ligikaudu 350 °C juures, mis viitab sellele, et vastuvoolu kasv ei korreleeru enam vastupinge kasvuga.