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Model implementation towards the prediction of J(V) characteristics in diamond bipolar device simulations

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ABSTRACT

In the view of predicting the performances as well as anticipating the architecture of the future diamond devices, it is of fundamental importance to accurately implement the physical properties of diamond into finite element based software. In this context, we used Silvaco to model a diamond p–n junction and studied the carrier densities responsible for the electrical characteristics of the devices. The simulated electrical characteristics are compared to experimental data and the influence of Shockley–Read–Hall and Auger recombination models on the carrier densities and J(V) characteristics was investigated. The bias voltage boundary between low and high injection conditions, $\Psi_{bi} = 4.7$ eV, was well reproduced. However, the extremely low calculated carrier densities lead to extremely low current densities in the low injection regime, reaching the numerical precision limit. The simulation of the reverse characteristic predicts a breakdown voltage of 225 V. Preliminary results on hopping conductivity implementation into the simulation tool are presented. Eventually, these results will be used to predict the architecture and behavior of future devices, such as bipolar junction transistor and metal–oxide–semiconductor field effect transistor.

Contents

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1. Introduction

The last twenty years of development in controlling both growth quality and doping concentration in CVD diamond has led to the emergence of electronic devices such as Schottky diodes withstanding high breakdown field (7.7 MV.cm^{-1}) [1], lateral p–n junctions with extremely low leakage current (<2.10^{-6} A.cm^{-2} under a reverse bias voltage of 30 V) [2], H-terminated field effect transistors showing high cutoff frequency (53 GHz) [3], junction field effect transistors using selectively grown n-type diamond having high current on/off ratios (10^{7}–10^{8}) [4] and more recently bipolar junction transistors fabricated either on (111)-oriented IIb diamond or (001)-oriented IIb diamond using the selective growth technique [5,6]. The physical properties of diamond, such as high breakdown field (10 MV.cm^{-1} [7]), high electron and hole mobilities (1000 cm^2.V^{-1}.s^{-1} and 2000 cm^2.V^{-1}.s^{-1} respectively, for doping levels below 10^{17} cm^{-3} at room temperature [8–10]), high thermal conductivity (22 W.cm^{-1}.K^{-1}) and extremely low intrinsic carrier concentration at room temperature ($n_i \approx 10^{-27}$ cm^{-3}) lead to the highest calculated figures of merit [11], making diamond the ultimate semiconductor for high power and high frequency electronic applications.

In this context, the prediction of the device electrical characteristics is needed in order to reach the predicted material limits. This prediction is possible by implementing the physical parameters and models of diamond in TCAD finite element based software. For instance, Rashid et al. [12] have modeled a 1D Schottky m–i–p+ diode and studied the forward and reverse J(V) characteristics of the structure. They presented the implemented models and pointed out the lack of data inherent to diamond material as well as the difficulties encountered to simulate intrinsic diamond layer since the intrinsic carrier concentration is of the order of 10^{-27} cm^{-3} at 300 K. They found good correlations between simulated and experimental Schottky diode J(V) characteristics. The architecture of such a unipolar device has also been studied in Ref. [13]. The authors studied the effect of a field plate on the electric field distribution in the structure showing the importance of numerical simulation for optimizing the device architecture. Nawawi et al. [14] modeled the static and transient characteristics of a diamond Schottky diode in order to demonstrate the potential of diamond unipolar devices for power electronic applications. However, a more systematic approach for modeling either unipolar or bipolar diamond devices is needed. Since diamond technology is still very young, there is a lack of parameter values in the numerical tools. In the perspective of accurately modeling diamond devices, it is of fundamental importance to implement the physical parameter values of diamond (impact ionization coefficient, carrier life-times) and mobility models into the device simulators, over a wide range of temperature. In this paper the physical parameter values of diamond have been implemented into Silvaco TCAD finite element based software. The implemented models have then been applied to a diamond p–n junction after Makino et al. [35] and Koizumi and Makino [33]. These references were used to compare the implemented parameter values and models.

In the first part of the present work, the numerical models will be described. Then, the simulated diamond p–n junction characteristics will be presented. The influence of temperature, Shockley–Read–Hall lifetimes and Auger recombination parameters on the carrier densities and on the J(V) characteristics will be shown. We will conclude on the perspectives and the main difficulties due to the lack of parameter values and models implemented in the numerical simulation tools.

2. Numerical models

Three models were used in order to take into account the specific properties of diamond, i.e. the incomplete ionization of dopants, the carrier mobility and the recombination processes.

2.1. Incomplete ionization

The free carrier concentrations are calculated by solving the neutrality equations:

$$p + N_d = \frac{N_a}{1+\frac{p}{\phi_a}}, \phi_a = g_h N_v T^{3/2} exp\left(-\frac{E_a}{kT}\right) \quad (1)$$

$$n + N_a = \frac{N_d}{1+\frac{n}{\phi_d}}, \phi_d = g_e N_c T^{3/2} exp\left(-\frac{E_d}{kT}\right) \quad (2)$$

where $p(n)$ is the free hole (electron) concentration, $N_{a(d)}$ is the acceptor (donor) concentration, $E_{a(d)}$ is the acceptor (donor) thermal activation energy, k is the Boltzmann constant, h is the Planck constant and T is the temperature. The effective densities of state are $N_v = 2(2\pi m_h^* k)^{3/2}/h^3$ and $N_c = 2(2\pi m_e^* k)^{3/2}/h^3$. The degeneracy factor is either $g_h = 1/4$ for holes or $g_e = 2$ for electrons [15] and the density-of-state effective masses are $m_h^* = 0.908\ m_0$ and $m_e^* = 0.55\ m_0$ for holes and electrons respectively. The hole density-of-state effective mass value is taken from Willatzen et al. in Ref. [16] and calculated by the procedure described by Pernot et al. in Ref. [10]. The electron density-of-state effective mass is calculated from the experimental values of Ref. [17] as $m_e^* = (m_\perp^2 m_{//})^{1/3}$, with $m_\perp = 0.306\ m_0$ and $m_{//} = 1.81\ m_0$. These implemented values are in close agreement with the recent experimental report of Naka et al. [18].

The large activation energies of dopants in diamond lead to incomplete dopant ionization at room temperature. This is the main reason why regular devices such as junction field effect transistor (FET) have poor electrical performances, and specific architectures have been developed such as delta-doped FET [19,20] or hydrogen-terminated FET [3]. As the physics leading to the reduction of the ionization energy is quite complex, an empirical law has been used, inspired from the Pearson and Bardeen model [21]. Parameters have been adjusted for boron acceptor in order to get 0.38 eV ionization energy at low dopant concentration [22] and zero at the insulator–metal transition of 4.5×10^{20} cm^{-3} [23]:

$$E_a(\text{eV}) = 0.38 - 4.7877 \times 10^{-8} \times N_a^{\frac{1}{3}} \quad (3)$$

where E_a(eV) is the thermal activation energy of the boron acceptor in electron-volt and N_a is the boron concentration in cm^{-3}. In the case of phosphorus donor, a constant value of $E_d = 0.57$ eV for the activation energy has been assumed [24,17] since reports indicate no measurable reduction up to 10^{19} cm^{-3}, and hopping conduction above. However, a recent report [25] indicates a decrease of the activation energy of phosphorus in the presence of high concentration of compensating impurities. In the present work, we only consider low compensated n-type diamond, thus the ionization energy of phosphorus is set to $E_d = 0.57$ eV.

It results that, at room temperature, about one acceptor in one thousand is ionized and only one donor in one million is ionized for a doping level of 10^{17} cm^{-3} (obviously lower values will be achieved when taking into account the compensation).

2.2. Empirical mobility model

Another parameter which influences diamond electronic device performances is the electron and hole mobility. The empirical model used to fit the experimental Hall effect measurements reported in Refs. [26,9] (see Eqs. (4) to (6)) has been implemented into Silvaco finite element based software via a built-in C language interpreter, in order to take into account the doping concentration and temperature dependence of the mobility. This method has been adopted, instead of the proposed Masetti model [27], in order to implement in a second time the hopping mechanism, presented in Section 5.2. The parameter values are summarized in Table 1.