Numerical study of Schottky diode based on single GaN NW on Si

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Abstract. Numerical modelling of Schottky diode formed by single GaN nanowire on Si substrate was performed. Two metals, namely, gold and platinum forming the Schottky barrier were considered. The potential barrier height was calculated taking into account occurrence of image force as well as Fermi level pinning at metal/semiconductor interface. Volt-ampere characteristics were obtained for different NW doping levels considering Wentzel–Kramers–Brillouin tunneling model. Cutoff frequencies are evaluated from current-time relaxation curves for different NW lengths and doping levels. It is shown that such diode structure demonstrates high-speed performance with cutoff frequency in the range from 0.1 to 0.9 THz for both studied metals.

1. Introduction
A large number of modern technical solutions are implemented with the use of high-speed electronics. First of all, it concerns mobile, wireless, satellite communications, local data transmission systems (Wi-Fi, Bluetooth, WiGig, WirelessHD), radar systems, medical diagnostic and therapeutic equipment. Current trends dictate necessity to reduce the size of electronic components and to increase their output power, speed, operating temperatures, resistance to radiation (spacecrafts). To achieve this, it is necessary to develop semiconductor devices based on materials capable to work in adverse conditions. One of the promising electronics materials is gallium nitride (GaN). Its properties (bandgap, critical breakdown field, electron mobility and saturation drift velocity) allow to significantly improve characteristics of semiconductor devices. The use of GaN nanowires (NWs) is an attractive way to achieve semiconductor devices high performance due to NW’s low crystal defects density and small footprint. Moreover, high crystal quality GaN NWs could be epitaxially grown on silicon that is more economically favorable than using expensive growth substrates such as GaAs, SiC or sapphire. For the last years the increase in investigations concerning devices based on NWs (for example [1–3]) is observed.

Schottky barrier diodes (SBD) is an essential part of high-frequency electronics because of its high operation rate, which is usually higher than that of p-n junction rectifiers. Also SBD has low turn-on voltage that is useful in power devices. This work is dedicated to the numerical calculation of the high-speed SBD based on single GaN NW on silicon substrate.
2. Calculation
In this work we used Comsol Multiphysics package to simulate the operating mode of a SBD based on a single GaN NW. The schematic picture of studied structure is shown in figure 1. GaN NW vertically positioned on n+ silicon substrate is approximated by a cylinder with diameter D_{NW} and length L_{NW}. Schottky barrier is formed at the top of NW between anode metal and n-GaN NW active region. The doping level of n+ Si substrate is assumed to be 10^{19} cm^{-3}. Such doping level was taken to reduce the series resistance. This feature is essential for achieving high cutoff frequencies.

There are several items that determine potential barrier height at metal/semiconductor interface. As it known the height of Schottky barrier in general depends on metal work function, semiconductor electron affinity and surface states density, the last usually is the main factor due to Fermi level pinning at the semiconductor surface. Thus, in our model this phenomenon was taken into account. The phenomenon of Fermi level pinning at GaN (0001) surface was reported by many authors, but reported experimental data slightly differ from each other. For example, M. Himmerlich et al. [4] reported on Fermi level pinning at 0.5-0.7 eV below conduction band minimum (CBM) at n-GaN (0001) surface. G. Cywinski et al. [5] found that in as-grown GaN this level is located at 0.48 eV below CBM. While G. Koley et al. [6] obtained this level to be at 1.4 eV below CBM for as-grown GaN and 0.6 eV for n+ GaN. Anyway, these results are in agreement with some theoretical studies, for example [7]. The estimations of GaN (0001) surface states density are also have some dispersion and according to, for example [6,8–10], are in the range from ~3·10^{11} to a several 10^{13} states/cm^{2}/eV. Thus, in this work we pinned Fermi level at 0.7 eV below CBM and assumed surface states density to be a constant at 10^{12} cm^{-2}eV^{-1} within the bandgap that is some average value of reported ones.

![Figure 1. The schematic view of modeled GaN NW SBD.](image)

One more phenomenon changing potential barrier height is the Schottky effect that was also included in our physical model. This phenomenon causes barrier lowering due to occurrence of image force [11]. The total barrier height was calculated according to Cowley and Sze [12].

The current transport across metal/semiconductor interface mainly carried out by majority carriers. There are four main types of charge transfer in contacts of this type with forward bias: thermionic emission, quantum-mechanical tunneling, recombination in the space charge region, and injection of minority carriers (holes in our case). With reverse bias, reverse processes take place (from metal to semiconductor). In our model thermionic emission transport as well as quantum mechanical tunneling were included. Tunneling effect was calculated considering Wentzel–Kramers–Brillouin (WKB)
approximation [13]. Also, in the general case, traps located near the metal/semiconductor interface can make a contribution to the total current; however, this process was not considered in this work.

The NW sidewall surface has surface states, that causes the depletion of the near surface layer. This leads to the NW conduction channel narrowing, which can directly affect the transport of carriers along the NW. In this work, the diameter of the NW was taken to be equal 200 nm. With this diameter, according to [14], the influence of the sidewall surface states on the NW conductivity is insignificant.

In this work two metals were considered as top electrode – gold and platinum. The work functions of gold and platinum were taken as 5.2 and 5.5 eV, correspondingly [15].

3. Results and discussion

Taking into account the image force as well as the presence of surface states, the magnitude of the Schottky barrier is voltage-dependent. Moreover, the higher the reverse applied voltage, the stronger the effect of barrier reduction. Figure 2 shows the dependence of the potential barrier height on the applied voltage calculated for various GaN NW doping levels.

![Figure 2(a, b). The calculated Schottky barrier height dependency on applied reverse voltage for gold (a) and platinum (b) contact.](image)

The observed barrier lowering allows easier charge carriers tunneling. And due to the fact that reverse current of Schottky diode exponentially depends on the barrier height, this leads to a significant increase in the reverse current at reverse biases. An increase in the NW doping leads to an even sharper decrease in the barrier height, which actually causes a decrease in the diode breakdown voltage. This effect is clearly seen on the volt-ampere (I-V) characteristics presented in figure 3. Note that, for the gold contact, compared to the platinum one, breakdown occurs at lower voltages. This is due to the fact that gold work function is lower by ~ 0.3 eV. Thus, the barrier height of the platinum contact is higher compared to gold (see figure 2). For the same reason the amplitudes of the currents for the gold contact with direct bias are higher at the same voltages (see figure 3).
To evaluate the frequency properties of the GaN NW/Si diode, the product of the structure series resistance \( R \) and its total capacitance \( C \) was determined for various GaN NW doping levels and NW lengths. Having the obtained \( RC \) constant, it is possible to determine the cutoff frequency of the diode, above which its efficiency essentially decreases. The expression for the cutoff frequency is [16]:

\[
\text{f}_{\text{cutoff}} = \frac{1}{2\pi RC}
\]

The \( RC \) constants were determined from the current-time relaxation curves after applying some small constant bias voltage \( \Delta U \) to the system. Before the bias was applied, the system was in a stationary state with an applied voltage \( U_0 \). For an RC-circuit, the analytical equation of current-time decay can be written as:

\[
I(t) = A\exp\left(-\frac{t}{RC}\right) + B
\]

where \( t \) - time, \( R \) – structure series resistance, \( C \) – structure total capacitance, \( A \) and \( B \) – constants. Here \( B \) is a direct current that flows through the diode at \( U_0 + \Delta U \) applied voltage. Figure 4 illustrates an example of calculated current-time decay curve and corresponding approximation.

Figure 3(a,b). (a) Modeled I-V curves for gold contact; (b) Modeled I-V curves for platinum contact.

Figure 4. The modeled current-time decay approximation for platinum contact. The NW length and doping level are 2 \( \mu \)m and \( 2 \times 10^{17} \) cm\(^{-3} \), correspondingly. \( U_0 = 0.5 \) V, \( \Delta U = 0.001 \) V.
Figure 5 shows the obtained dependences of the cutoff frequency on the NW length and its doping level \( (N_d) \). For both gold and platinum contacts, with an increase in the NW length (at fixed doping level) a decrease in the cutoff frequency is observed. This appears due to an increase in the series resistance of the structure. Thus, to increase the cutoff frequency, a minimum NW length is required. However, it should be noted that a parasitic capacitance shunting the diode due to the presence of the top and bottom electrodes will inevitably be present in the real structure. At small NW length this capacity will be decisive, while the smaller the length, the greater the capacity. This will lead to a significant decrease in the cutoff frequency. We estimated the minimum NW length (not presented at this work) at which the parasitic capacitance would not significantly affect the frequency properties to be 2 µm.

Figure 5 (c, d) show the cutoff frequency as a function of NW doping for the 2 µm NW length. It is clearly seen that with the increase in doping level the cutoff frequency increases. In this case, both for the gold and platinum contacts, the cutoff frequency lies in the range from 0.1 to 0.9 THz.

Figure 5. (a) Calculated cutoff frequency for gold contact as a function of NW length; (b) Calculated cutoff frequency for platinum contact as a function of NW length; (c) Calculated cutoff frequency for gold contact as a function of NW doping; (d) Calculated cutoff frequency for platinum contact as a function of NW doping.

4. Summary
In this work, numerical modeling of the operating mode of the single GaN NW-based SBD diode was performed. The Schottky barrier height was calculated as a function of reverse voltage taking into account image force and surface states density at a metal/semiconductor interface. For the different
values of GaN NW doping levels the I-V curves were obtained. The cutoff frequency was estimated as a function of NW doping level and length. It is shown that NW length increase causes cutoff frequency reduction, while NW doping increase leads to cutoff frequency raise. For both gold and platinum contacts the cutoff frequency is in the range from 0.1 to 0.9 THz.

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