Modeling the semiconductor devices with negative differential resistance based on nitride nanowires

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Abstract. We proposed a numerical model of the Gunn diode and resonant diode based on a single nitride nanowire. Important model parameters needed for development of the considered devices, namely layers thickness, composition and doping level were evaluated. It has been shown theoretically that the single GaN nanowire based Gunn diode is capable to operate in over 1 THz frequency regime.

1. Introduction

Semiconductor nitride compounds are very promising for developing up-to-date high efficiency electronic devices. The most commonly used in device production nitride compounds are InN, GaN, AlN and their solutions (known as III-N). Due to high electron mobility and thermal conductivity nitride materials are good candidates for use in radio frequency (RF) power devices such as RF FET, Gunn diode and other.

The Gunn diode is an RF current generator which operation is based on non-linear dependence of electron velocity on electric field in the material. This dependence leads to negative differential resistance regime when specific voltage is applied. The most successful devices of this type are based on GaAs and can emit waves with frequency up to 100 GHz. Theoretically, use of nitride semiconductors allows to extend this range over 1 THz due to fast interband transitions and large critical electric field.

There are several technological problems in production of III-N based planar devices, probably main of them is absence of lattice-matched substrate. Another important problem is piezoelectric field along c-direction caused by the wurtzite crystall structure. The first point limits crystal quality and therefore mobility, efficiency and maximum operation frequency of the devices while the second point makes inapplicable many common successful designs. Use of nitride nanowires allows, firstly, to improve the device crystal quality and, secondly, to select nonpolar crystal direction. One important feature about the III-N nanowires is a variety of applicable growth techniques such as metal-organic...
chemical vapour deposition and molecular beam epitaxy, as well as variety of growth substrates including sapphire, silicon, polished metal wafers and some other [1].

2. Modeling
In this work we considered model of Gunn diode based on a single GaN nanowire with modulated doped layers in polar directions. The calculation was done in Silvaco TCAD program. The majority of bulk semiconductor parameter values were taken from [2], while the mobility value of MOCVD GaN nanowires was taken from [3].

It is known that Gunn effect can be observed in materials that have negative differential mobility in high electric fields. In such case, high electric field mobility depends on ionized impurity concentration as well as temperature. Experimental measurement of this dependence is a difficult task due to need of many structures fabrication differing with doping level as well as necessity to carry out time resolve volt-ampere measurements to register the Gunn effect.

Instead of experimental measurements, we have calculated electron velocity dependence on electric field along the Monte Carlo method which is often used for this purpose. Carrier differential mobility can be found as derivative of electron velocity on electric field. In our electron velocity calculation we took into account ionized impurity scattering and intervalley phonons. In figure 1 one can see the calculated dependence of electron velocity on electric field for different NW doping levels under 300 Kelvins. The calculations show us that electron velocity decrease takes place for doping level under 10^{19} cm^{-3}, but not for 10^{20} cm^{-3}. This might be an identification of threshold doping concentration existence around 10^{19} for Gunn effect in case of GaN NW.

![Figure 1. Monte Carlo simulation of electron drift velocity in GaN for different doping levels.](image)

Results of the Monte Carlo simulation were adapted to TCAD negative differential mobility model to study numerically Gunn effect in GaN NWs [4]. We should mention here, that method above is applicable to calculate high electric field behavior of GaN NW conductivity but not for low field one.

In the calculations we considered single GaN NW with typical for MBE parameters: diameter (D) of NW was 200 nm, active region thickness (H_{AO}) was from 200 to 2000 nm and the doping level of active region was from 10^{17} to 10^{19} cm^{-3}. Existence of the surface states (N_{SS}) in GaN was also taken into account. Energy level of the surface states in GaN was considered as 0.6 eV and their density about (1-2)10^{11} eV^{-1}cm^{-2}[5]. Figure 2(a) shows schematic image of the NW model. Emitters in the model were assumed GaN with 10^{19} cm^{-3} doping level and 50 cm^{2}/(V·s) fixed mobility. Anode and cathode were assumed metallic with total resistance of 25 Ohm each.
Figure 2(a, b). Schematic image of GaN NW model (a) and electron density waves in NW due to Gunn effect (b).

In our Gunn effect numerical simulation we calculated time resolve volt-ampere characteristic for each set of model parameters. Simulated voltage was applied with linear ramp from zero to $V_{\text{max}} = E_{\text{max}} / H_{\text{AO}}$, where $E_{\text{max}}$ is maximum electric field value for active region of specified thickness. The ramp time and stabilization time were 100 ps each. Stabilization time is needed to steady the current oscillations induced by Gunn effect. After stabilization of the simulated oscillations the program calculated them for 50 modeled ps to obtain percentage of RF signal among all the current through NW and to make Fourier transform in order to obtain frequency dependence instead of time dependence. To obtain RF current percentage, standard deviation of oscillating current was calculated and divided by mean current value.

Figure 3(a, b). RF current part dependence on: (a) anode-cathode voltage drop, (b) one of active region thickness.

Figure 3(a) shows RF current part dependence on applied voltage between anode and cathode for different surface states density. According to the calculation results surface states lead to energy bands bending what reduces the electron concentration near NW edge. This phenomenon works as an effective decrease of the NW diameter. Readers can see electron domains as well as reduction of the electron concentration inside the domain edge in figure 2(b). Electron domains consist of heavy electrons from non-gamma valleys. The thickness of electron domains correlates with electron density.
If the active region thickness is smaller than the domain thickness then the Gunn diode efficiency will be reduced similar to fall of the RF current part with decrease of active region thickness in figure 3(b).

Fourier transform of the current oscillations data allows to distinguish higher order modes from the first mode. According to the calculations oscillation frequency decreases with active region thickness increase as shown in figure 4(a). This phenomenon is intuitively understandable as current oscillation period is a time between two consecutive acts of domain formation. One domain drifts to anode with saturation velocity of heavy electrons which is fixed for specific doping level. So when the thickness decreases the oscillation time decreases too.

Figure 4(a, b). Current oscillation spectra in Gunn diode for different applied voltages and active region thickness.

As it shown in figure 2(b) there is a distance between cathode and the first electron domain. In this region electrons accelerate until they obtain enough energy to become heavy electrons which form the domains. The lower applied voltage, the lower electric field in the structure, so the thickness of the acceleration region is higher. For this reason, the domain thickness should be not more than active region thickness minus thickness of this region which leads to increase of the oscillation frequency with decrease of the voltage as it shown in figure 4(b).

In spite of possibility to increase the oscillation frequency by decreasing the active region thickness and increasing the doping level there is a critical frequency value for the material. The first reason for that is existence of the critical electron density in domain that depends on critical electric field (point of maximum velocity)[6]. The critical electric field related to energy difference between gamma-valley and a second valley. So, for GaAs this difference is about 0.29 eV, but for GaN it is more than 1.1 eV. The second reason is existence of the impulse relaxation time for the material. This is time needed to form the electron domain. Thus, the way to increase the oscillation frequency is use of material with lower impulse relaxation time and higher critical electric field.

3. Summary
We shown theoretically that specially designed nitride NW can act as an RF device despite existence of the surface state level. We demonstrate that Gunn diode based on single GaN NW is able to operate in a frequency range over 1 THz.

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