Turk J Phys
28 (2004) , 369 – 377.

Simulation of Millimeter-Wave Gunn Oscillations in Gallium Nitride

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Received 20.07.2004

Abstract

High field transport in wide bandgap semiconductors like GaN is of great technological importance. The negative differential mobility regime at high fields, under suitable conditions, can lead to millimeter-wave Gunn oscillations. Using extensive simulation based an ensemble Monte Carlo technique, the prospects of GaN Gunn diodes are theoretically investigated. The possibility of operating these Gunn diodes at their higher harmonic modes are explored. The main finding of this research is that the carrier dynamics in GaN can be tailored by an optimum choice of doping profile, temperature and bias conditions so that the efficiency of higher harmonic Gunn oscillations can be boosted. Finally, the physical origin of these Gunn oscillations is sought exploring whether it is the intervalley scattering mechanism, the Γ valley nonparabolicity, or the effective mass discrepancy between the Γ and the lowest satellite valleys as the responsible mechanism.

1. Introduction

At high electric fields, the electron velocity v in GaAs, GaN, InP, and most other III–V compound semiconductors, decreases with an increase in the electric field F so that the *differential mobility* $\mu_d = dv/dF$ becomes negative. Ridley and Watkins in 1961 and Hilsum in 1962 were first to suggest that such a *negative differential mobility* in high electric fields is related to an electron transfer between different valleys of the conduction band (intervalley transfer). When the electric field is low, electrons are primarily located in the central valley of the conduction band. As the electric field increases, many electrons gain enough energy for the intervalley transition into higher satellite valleys. The electron effective mass in the satellite valleys is much greater than in the central valley. Also, the intervalley transition is accompanied by increased electron scattering. These factors result in a decrease of the electron velocity in high electric fields. There are mechanisms other than the intervalley transfer to achieve negative differential mobility, such as the Γ valley nonparabolicity. As of great technological importance, when such materials are operated in their negative differential mobility regions, regenerative instabilities are created, causing charge bundles, termed as Gunn domains, traveling along the structure. Hence, this can be utilized as solid-state microwave or millimeter-wave generators.

Gallium nitride with its high negative differential mobility threshold, measured [1] to be above 200 $\mathrm{kVcm^{-1}}$, is an appealing material for high power millimeter-wave Gunn diodes [2, 3]. An ever-present objective is to increase the operating frequency of the Gunn diodes, and a promising approach is to operate them at their higher harmonic modes rather than their fundamental mode. Recently, a number of researchers [4, 5, 6, 7, 8] focused on this point addressing the dependence of the higher harmonic efficiency on the doping profile, mainly referring to the mature InP technology. The literature on GaN based Gunn diodes has not yet flourished, as the research community up to now has mainly focused on the perfection of the material growth quality as well as laser and heterojunction bipolar transistor applications [9]. Among the recent theoretical reports published on GaN Gunn diodes, Joshi et al. studied multiple-transit region effects on the output power [10], Lü and Cao analyzed chaotic dynamics in terahertz generation [11] and Gruzinskis et al. considered the Gunn diodes with the zincblende phase of GaN and also wurtzite phase GaN structures with a p-doped barrier region to achieve current reduction [12].

In this work, our aim is to present a comprehensive theoretical assessment of efficiency and harmonic enhancement in n-type GaN Gunn diodes, exploring the effects of including a doping notch/mesa, channel concentration, DC bias and the lattice temperature. We would like to extract the *trends* rather than quantitative aspects so that our results can shed light on the physics of millimeter wave Gunn oscillations based on other materials as well. We employ the ensemble Monte Carlo (EMC) technique which has been previously successfully tested in the analysis of InP Gunn diodes [13].

2. Structural and Computational Details

In a similar work on GaN, Joshi et al. [10] used the energy of the lowest satellite valley with the U point 2.2717 eV above the conduction band minimum, which we also followed in our subsequent work [14]. As for the current work, we use a more realistic bandstructure data (see Figure 1) that places the U valley 1.34 eV above the conduction band minimum [10]. All major scattering mechanisms are taken into account, while the scattering tables are formed based on the pseudopotential density of states of GaN. For further details of the parameters, we refer to our previous work on avalanche photodiodes [16, 17].

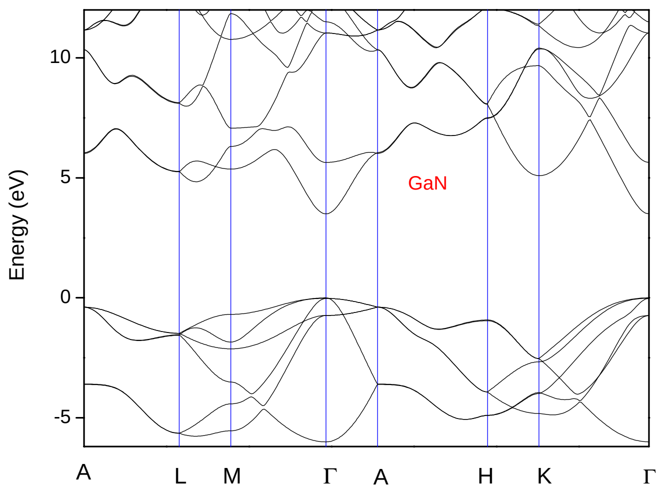

Figure 1. Empirical pseudopotential band structure of Gallium Nitride.

The types of GaN-based Gunn structures we study are shown in Figure 2. The overall active region length is always kept constant at a value of $l_a = 1.2$ μm. This active region is sandwiched between the heavily doped n^+ regions with $n^+ = 2 \times 10^{18}$ cm^{-3}; the results were seen to be unaffected when this is increased to 1×10^{19} cm^{-3}. The active region is composed of an active channel with a doping of $n = 3 \times 10^{17}$ cm^{-3} (unless stated otherwise) and a lightly n-doped doping notch having $n^- = 1 \times 10^{16}$ cm^{-3} or a doping mesa with $n^+ = 5 \times 10^{17}$ cm^{-3}.

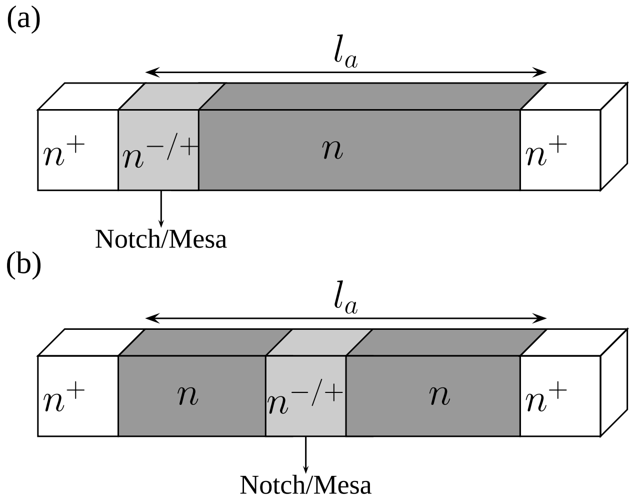

Figure 2. The types of GaN-based Gunn structures studied: (a) Notch/mesa placed next to cathode, (b) Notch/mesa placed in the middle of the active region.

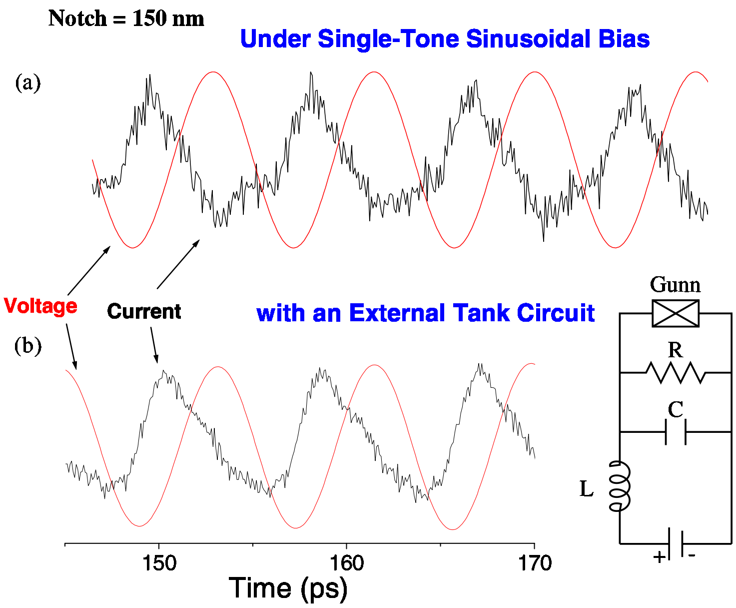

Figure 3. Current and voltage waveforms for a 150 nm-notch Gunn diode (a) under an imposed single-tone sinusoidal voltage, and (b) connected to an external tank circuit shown in the inset.

Our EMC simulations start from a charge-neutral configuration, and unless otherwise stated, are at 300 K. As a standard practice in modeling Gunn diodes (see Ref. [7] and references therein), a single-tone sinusoidal voltage of the form $V_{\rm DC} + V_{\rm AC}\sin(2\pi ft)$ is imposed across the structure; if not stated, we use $V_{\rm DC} = 60$ V and $V_{\rm AC} = 15$ V. This choice significantly simplifies our frequency performance assessment. Moreover, its validity was checked by relaxing the imposed single-tone sinusoidal voltage across the Gunn diode and connecting it to an external tank circuit with the voltage across the device being self-consistently updated at each simulation step through solving the Gunn diode and the external circuit (c.f. Figure 3).

For both cases, the phase relations were found to be very similar [14]. In these simulations more than 25,000 superelectrons have been employed, and at least 0.2 ns is simulated to assure that both amplitude and phase have stabilized. The current waveform is sampled at every 80 fs while the simulation time step is 0.4 fs.

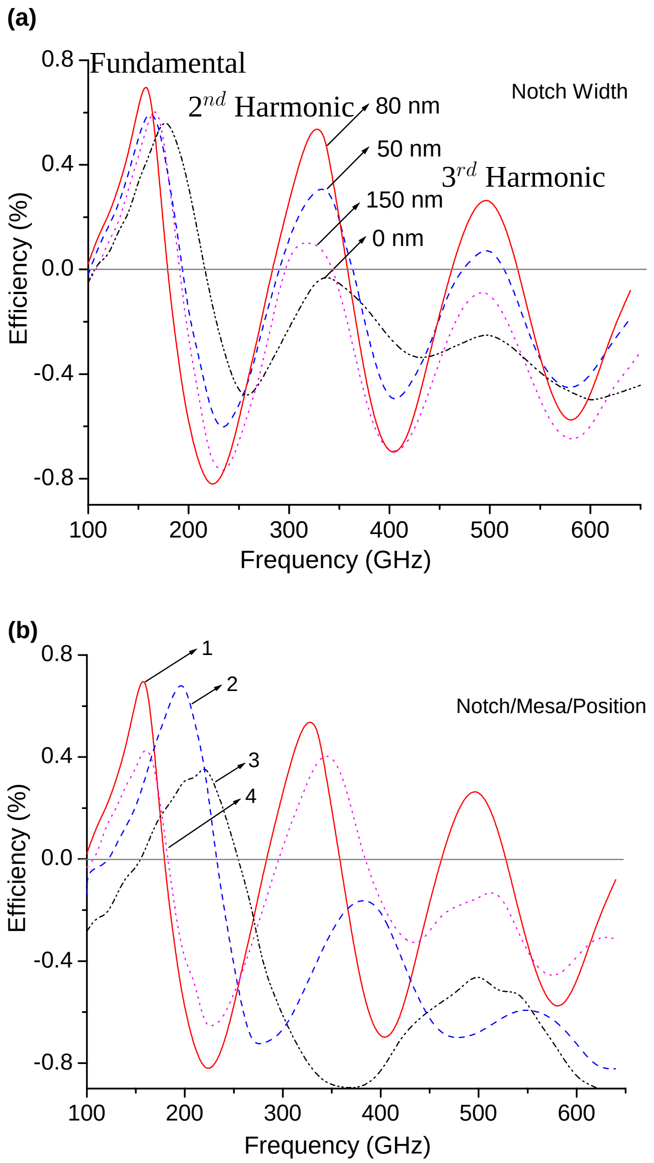

Figure 4. (a) Effect of different doping notch widths, (b) Comparison of the performance of four configuration made from the combinations of notch/mesa placed next to cathode and in the middle of the active region, while keeping the notch/mesa = 80 nm. 1→notch next to cathode, 2→mesa next to cathode, 3→notch in the middle of the active region, 4→mesa in the middle of the active region.

3. Results

The quantity of primary interest, oscillator efficiency, is defined as $\eta = P_{\mathrm{AC}}/P_{\mathrm{DC}}$, where P_{AC} is the time-average generated AC power and P_{DC} is the dissipated DC power by the Gunn diode. First, the effect of the doping notch width (positioned next to cathode, c.f. Figure 2a) is investigated. It is observed that there is an optimum notch width, for our case, around a value of 80 nm, at which the second harmonic efficiency approaches that of the fundamental mode value as seen in Figure 4a. Here, the fundamental mode corresponds to the frequency $v_{d,sat}/l_a$ for a given active region length l_a, where $v_{d,sat}$ is the saturation drift velocity. In the $n^{\rm th}$ harmonic mode, there exist n Gunn domains traveling down the channel at each instant (see Figure 5). However, we would like to point out that the value of the optimum notch width is sensitive to the material parameters and our previous analysis with the bandstructure data of Ref. [10]. resulted in a wider width [14]. On the other hand, a doping mesa rather than a notch was suggested to enhance the harmonic content of the current waveform [4, 6]. To elucidate this point, Figure 4b compares the performance of four configurations made from the combinations of notch/mesa placed next to the cathode and in the middle of the active region. It is seen that notch placed next to the cathode (labeled as 1) performs the best among all. A source of curiosity regarding Figure 4b is the substantial frequency shift for the notch placed in the middle (labeled as 3) and mesa placed next to the cathode (labeled as 2). Detailed investigation of these structures shows that for both cases almost half of the active region is inactive in the domain nucleation processes, hence remarkably decreasing the transit time of the Gunn domains.

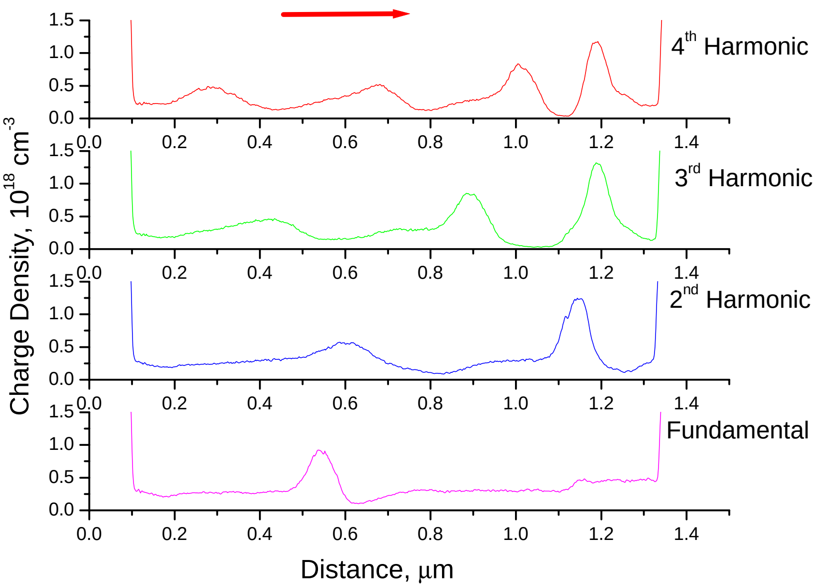

Figure 5. Typical traveling charge density profiles for a device operating at the fundamental, second, third, fourth harmonic modes.

In Figure 6 the effects of DC bias and channel doping are displayed. While changing the applied DC voltage across the Gunn diode we need to scale the RF amplitude accordingly so as not to lose the grounds for efficiency comparison. The applied DC voltage has to be above a critical value so that the device is biased in the negative differential mobility regime. Therefore, increasing bias has favorable effect on the fundamental and harmonic efficiencies. The channel doping, on the other hand, is relatively, less influential on the fundamental mode efficiency than the higher harmonic modes, so that for a given notch width and bias voltage, there is an optimum channel doping that favors the harmonic enhancement. However, there is a lower threshold for the channel doping, as it determines the dielectric domain nucleation time, a time that needs to be much shorter than the domain transit time through the active region [18].

For high power Gunn diodes, thermal heating can be an important issue. At the expense of neglecting thermal gradient effects, we simply consider the uniform lattice temperature effects on the efficiency. As

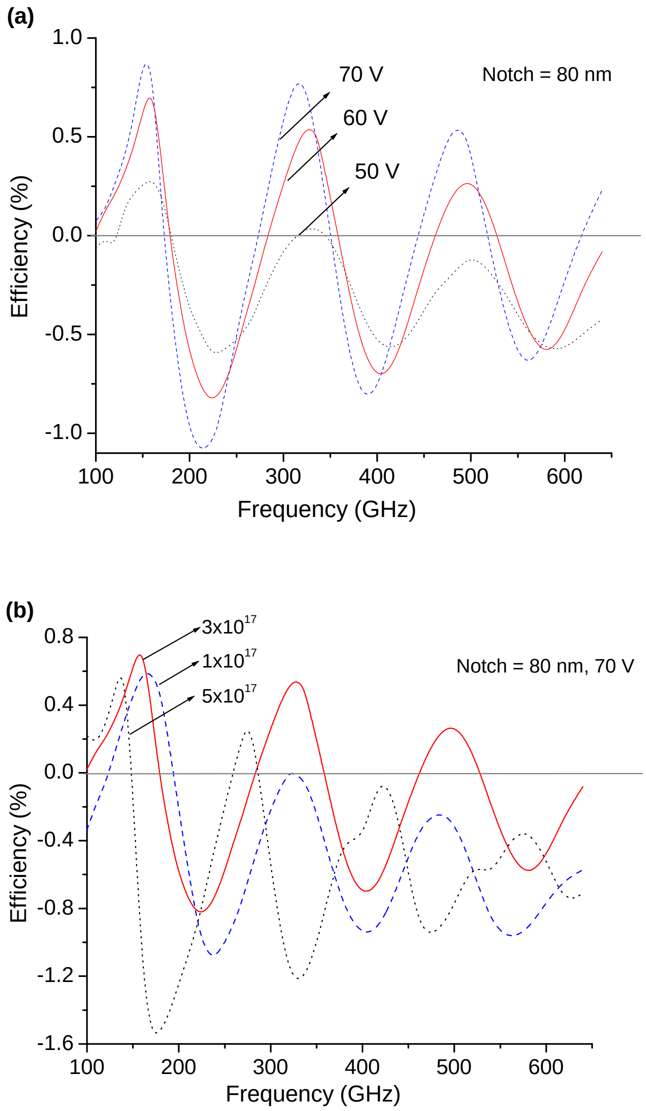

Figure 6. RF conversion efficiencies versus frequency for several DC bias voltages with the RF amplitude being scaled accordingly; 80 nm-notch device.(b) RF conversion efficiency versus frequency for channel dopings; 80 nm-notch device at 70 V DC bias is used.

can be observed in Figure 7a, up to room temperature there is no sensible variation, whereas above room temperature performance increasingly degrades, becoming passive above 480 K in the case considered. The source of this degradation is not due to a reduction in the oscillation amplitudes, but rather due to phase angle between the current and voltage waveforms shifting away from anti-phase (180°) to orthogonal (90°) and to dissipative (0°) as the temperature increases. As a matter of fact, the phase angle difference is always far below 180° due to the finite capacitance of the Gunn diode, which is not canceled by an external inductor under the imposed single-tone sinusoidal bias condition that is employed in this work. Figure 7b further illustrates that the increase in the lattice temperature does not significantly shift the frequency but diminishes the efficiency globally. Therefore, good heat sinking is required in these GaN Gunn diodes.

On the physical origin of the Gunn oscillations, there exists a number of possible sources; such as the Γ valley nonparabolicity; intervalley transfer mechanism to satellite valleys; and as recently suggested [11],

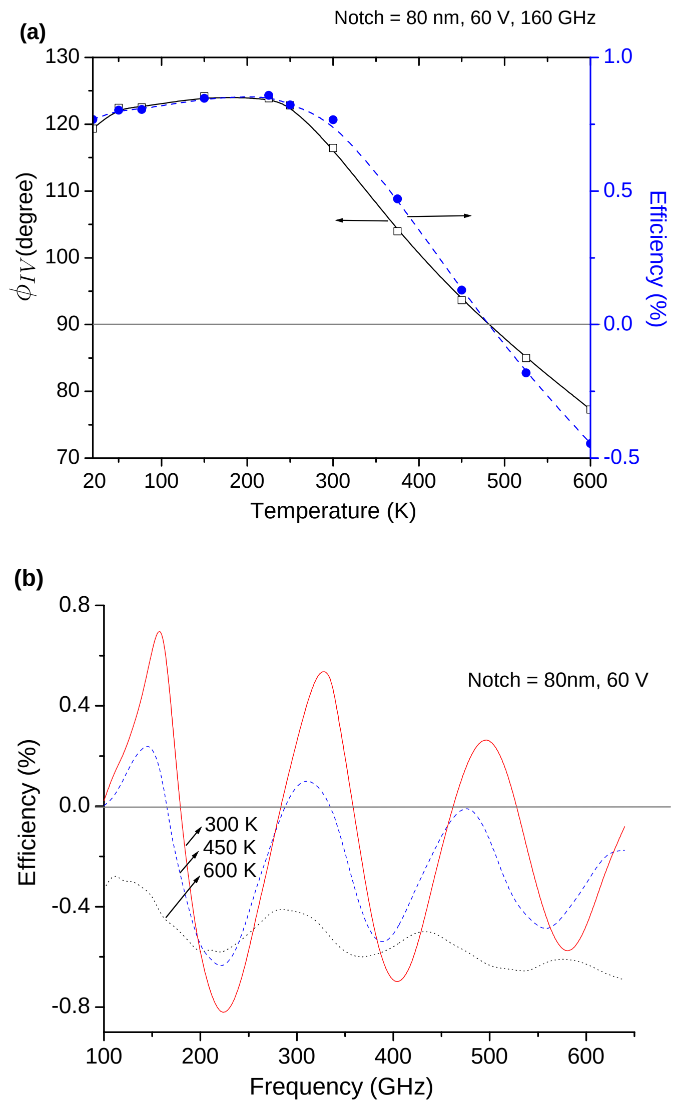

Figure 7. (a) Temperature versus phase angle between the current and voltage waveforms, and efficiency; 80 nm-notch device at 60 V bias and its fundamental frequency (160 GHz) is used. (b) RF conversion efficiency and frequency for several lattice temperatures; 80 nm-notch device at 60 V bias is used.

ballistic transport through the Γ valley band inflection point when located below the lowest satellite valley energy. In our EMC treatment, based essentially on monotonically increasing bands, hence without any band inflection points, this last choice cannot play a role. To characterize the effect of Γ valley nonparabolicity, switching to a parabolic band further increases the RF generation efficiency, whereas increasing the nonparabolicity decreases it. This rules out the fact that it can be the cause; and one can reason it by arguing that the nonparabolicity delays the electrons, under the electric field's acceleration, from reaching the satellite valley energy. On the effective mass discrepancy, the lowest satellite U valley is more than twice as heavy as the Γ-valley [19], which advocates the transfer from a light to a heavy band as an additional driving mechanism. Interestingly, equating these two masses decreases the the efficiency somewhat but it does not quench it. As a matter of fact, we identified the optical deformation potential field which leads to intervalley scattering as the most important parameter that controls the efficiency. Fortunately, its value for GaN has recently been rigorously determined by Akis et al. [20].

4. Conclusion

In summary, we have analyzed the trends in efficiency and harmonic enhancement in GaN Gunn diodes under doping profile, bias and temperature variations. The key parameter in all these efficiency considerations has been the phase angle difference between the current and voltage waveforms. Our extensive simulations indicate that the carrier dynamics in GaN can be tailored by an optimum choice of doping profile, temperature and bias conditions so that the efficiency of higher harmonic Gunn oscillations can be boosted.

Acknowledgment

This work has been supported by The Scientific and Technical Research Council of Turkey (TÜBİTAK) under the COST288 action.

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