ABSTRACT

BARRY, EDWIN A. Terahertz Generation in Submicron Nitride-based Semiconductor Devices. (Under the direction of Dr. Ki Wook Kim).

In this thesis, the electron dynamics and transport properties of III-nitride semiconductor materials and devices are studied, with an emphasis on their application to the generation high-frequency electromagnetic radiation. Numerical simulation models, including Monte Carlo, drift-diffusion, and thermal diffusion are utilized to model transport in the hot-electron and moderate-field regimes.

The Monte Carlo method is first applied to the study of the distribution function and the basic characteristics of hot electrons in III-nitrides under moderate electric fields. It is found that in relatively low fields (of the order of kV/cm) polar-optical phonon emission dominates the electron kinetics giving rise to a spindle-shaped distribution function and an extended portion of a quasisaturation of the current-voltage (I-V) characteristics.

The Monte Carlo program developed for the study of the III-nitrides is then extended to include the quantum mechanical spin evolution of electrons in bulk GaAs at room temperature. The spin relaxation time and characteristic decay lengths of spin polarized electrons are determined.

Next, the conditions for microwave power generation in a submicrometer GaN diode are investigated. By applying a high-field electron transport model based on
the local quasistatic approximation, it is shown that oscillations in GaN diodes can be supported in the terahertz-frequency range near the LSA regime. The shape of the diode voltage and electronic current waveforms are examined in terms of the circuit parameters and operating frequencies over the bandwidth of active generation. Based on a Fourier series analysis of the diode voltage and current, the generated power and dc-to-RF conversion efficiency at the fundamental and the lowest higher harmonic frequencies are estimated. The calculation results clearly indicate that submicrometer GaN diodes (channel doping of $1 \times 10^{17} \text{cm}^{-3}$) can achieve large output powers ($> 1 \text{ W}$) in the absence of Gunn domain formation, over a wide range of frequencies, near 0.5 terahertz.

Finally, conditions for pulsed dc regimes of terahertz power generation are theoretically investigated in a vertical nanoscale $n^+nn^+$ GaN-based diode coupled to an external resonant circuit. A combined electrothermal model is adopted allowing for a detailed analysis of the dynamical local distributions of the electric field, drift velocity, and lattice temperature via self-consistent simulation of the high-field electron transport in the active channel and the thermal transport in the device structure. The main performance parameters including, generation power, efficiency, and operation frequency are determined for stable generation with short pulses of a few ns and a few tens of ns of duty cycle. The presented results can be used for optimization and design of two-terminal GaN-based high-power THz generators for pulsed regime operation.
Terahertz Generation in Submicron Nitride-based Semiconductor Devices

by

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DEDICATION

To my parents.
BIOGRAPHY

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Chapter 1

Introduction

1.1 Overview

The generation and detection of electromagnetic radiation in the terahertz (THz) frequency domain is of growing interest in recent years [1]-[5]. This is due to a large variety of potential applications such as biological and medical imaging [6], sensing for security target screening [7, 8], chemical and solid-state spectroscopy, etc. [9] While there are several successful avenues for the generation of THz radiation [10]-[13], compact solid-state THz oscillators capable of operating at room temperature and delivering output powers on the order of or greater than tens of milliwatts are of at the center of attention [14]. The development of an efficient and practical means of THz generation remains elusive despite large scale focused research efforts. Part of the difficulty, with regard to a solid-state method of generation, is due to the specific
characteristics of common semiconducting systems. The microwave frequency range, which falls below the THz range, and the near infrared frequency range above are already well utilized. However, current solid-state microwave devices, which depend on the usual characteristic time scales of carrier transport, have reached their high frequency limit of a few hundred gigahertz. At the same time, the frequency range of solid-state devices which depend on interband transitions are limited by the size of the band structure energy gap. This corresponds to a lower limit of approximately 10 THz and leads to a large and undesirable gap in the usable electromagnetic frequency spectrum [3].

By exploiting the unique transport properties of wide-bandgap semiconducting materials in novel and unconventional devices it is possible to bridge the “THz gap” with compact and highly integrable solid-state configurations. Specifically, the properties of group-III nitride semiconductors [9]- [15], including a large bandgap for high power generation and high breakdown electric fields, make them promising candidates. Large electron drift velocities (leading to short transit times) and strong electron-polar optical phonon coupling (leading to very short characteristic scattering times) make the nitrides favorable for high-field transport induced negative differential resistivity (NDR) [16].

The large variety of applications, including biological and medical imaging, solid state spectroscopy and those pertinent to the military make THz technologies a relevant and promising area. The manipulation of electronic instabilities in submicron
semiconductor structures offers promising solutions to fill the current void of sources of THz electromagnetic radiation. The main goal of this work is to characterize and model a convenient and integrable submicron semiconductor THz source based upon the negative differential resistance effect present in gallium nitride (GaN).

1.2 Streaming Regime in III-nitrides

In Chapter 2, the results of a Monte Carlo simulation of III-nitride semiconductors in the streaming regime are presented. The model is used to analyze the carrier dynamics and highly anisotropic electron distribution function due to the dominance of polar optical phonon scattering at low temperatures. The properties of the streaming regime are first defined, followed by details of the simulation method. An analytical description of the conditions for streaming are given. The transport characteristics of the average drift velocity, the average kinetic energy associated with electron motion transverse to the field, and the mean-square deviation of the longitudinal component of the electron velocity are then calculated and examined.

1.3 Monte Carlo Simulation of Spin Relaxation

In Chapter 3, the traditional Monte Carlo method used in the simulation of electronic transport is extended to include a description of the evolution of the quantum mechanical electron spin. The mechanisms for the spin relaxation of a polarized distri-
bution of electrons are defined and included in the simulation model. Spin-dependent transport in bulk gallium arsenide (GaAs) in the drift regime is investigated and the spin relaxation time and characteristic decay lengths at room temperature are determined.

1.4 Simulation of Terahertz Generation in Submicron GaN $n^+nn^+$ Diodes

In Chapter 4, the conditions for the terahertz operation of a submicron $n^+nn^+$ GaN diode are investigated by the drift-diffusion method. A nonlinear analysis and numerical simulation the diode, coupled to an external resonant circuit, is made and conditions for the operation of the diode near the limited space charge accumulation (LSA) mode are described. A quantitative evaluation of the main performance parameters including output power, efficiency, and operating frequency, as well as the higher-order harmonic contributions to the generated THz signal, is made. The external circuit is tuned, by adjusting the bias voltage and load resistance, and the frequencies for which generation is possible are analyzed.
1.5 Electrothermal Simulation

In Chapter 5, the effects of temperature degradation on the output performance of the pulsed mode operation of a n-GaN NDR diode THz generator are reported. The diode is combined with a parallel RLC resonant circuit to establish stationary oscillations and the self-heating effects due to Joule heating in the conducting channel are studied. The dynamic temperature distribution in the diode channel and device substrate are calculated and the effect of self-heating is incorporated by self-consistently updating the temperature dependent electron drift velocity in the drift-diffusion model. A quantitative appraisal of the diode operation parameters including dc-to-RF conversion efficiency, ac generated power, temperature distribution and operating frequency are given.

1.6 Concluding Remarks

In Chapter 6, the results of the previous studies are summarized and suggestions for future work are presented. Recommendations for enhancements of the current models are offered in addition to modifications of the device design which may lead to the improved performance of n-GaN NDR diodes at increased frequencies. Specifically, the extension of the Monte Carlo simulations used in the first two chapters to include thermal effects will allow the analysis of even shorter diode channel lengths, possibly offering larger operating frequencies above 1.0 THz.
Chapter 2

Monte Carlo Simulation of the

Streaming Regime in III-nitrides

2.1 Introduction

The wide range of potential applications for THz electromagnetic radiation have provided an impetus for the development of efficient integrable semiconductor sources [1]-[3]. Various potential devices have been studied, both theoretically [15]-[21] and experimentally [16], [22]-[26], which seek to utilize novel transport properties to extend their frequency of operation. Historically, in the generation of microwave radiation, III-V based devices have been extensively used, due to the inherent non-linear characteristic of the materials electron drift velocity response to an applied electric field [27].

In recent years, III-nitrides have been attracting more and more attention. Indium
nitride (InN), aluminum nitride (AlN), gallium nitride (GaN), and their alloys are generally characterized as wide bandgap semiconductors, with energy gaps between 2.0 eV and 6.0 eV [28]. They have been utilized extensively in optoelectronic applications since they have direct band gaps which support generation in the blue and ultraviolet bands of the electromagnetic spectrum. This was a long sought after portion of the electromagnetic spectrum, unattainable with devices based on previously used semiconductor systems.

The III-nitrides also have high critical electric breakdown fields, a property attributed directly to their large band gaps. In high fields, as the process impact ionization begins, secondary carriers are generated initiating the process of breakdown [29]. The impact ionization threshold is approximately proportional to the size of the bandgap. Therefore, in most cases, the breakdown voltage will increase as the bandgap increases and vice versa. This allows for the design of nitride-based power devices which operate at higher voltages than were previously possible.

One of the other favorable properties of the III-nitrides, and wide bandgap semiconductors in general, are their high thermal conductivities which enable operation at high current densities and in applications with high thermal stress [30]. Additionally, their high peak and saturation electron velocities make them quite favorable for high speed applications. GaAs-based devices have traditionally been used for the successful generation of high frequency microwave electromagnetic generation extending from the UHF to the W-band frequencies. Three terminal InP and GaAs heterojunc-
tion bipolar transistors (HBTs) [31] and high electron mobility transistors (HEMTs) are prevailing high frequency power sources [32]. The drift velocity vs. electric field characteristics are shown schematically in Figs. 2.1 and 2.2 for GaAs and GaN, respectively. Therefore, the larger drift velocities in the nitrides can be expected to produce faster operation in similar device configurations.

Comprehensive theoretical and experimental studies have been conducted in GaAs, silicon (Si), and many other semiconductors. Among the most valuable of the theoretical models is the Monte Carlo semiconductor device simulation [33]-[37]. The detailed electron and hole transport physics, which determine the behavior of submicron devices, have extensively studied in the literature. Developed by a number of groups, ensemble full-band simulations have given insight into the underlying phenomena responsible for device performance.

The semiclassical Boltzmann transport equation can be used to describe the carrier dynamics both bulk semiconductors and semiconductor devices [38]. The solution of this equation is usually quite cumbersome and a number of methods have been employed. The stochastic Monte Carlo method has proven to be an accurate technique which supplies a satisfying intuitive approach which may include details of the system including full band structure, applied fields, the geometry of devices, and numerous scattering mechanisms. This technique, widely use to investigate transport in III-nitrides [39]-[42], is used below to investigate the moderate field electron dynamics known as the streaming regime.
Electric Field (kV/cm) vs Drift Velocity (x $10^7$ cm/s)

- Electric Field ($E_C$) ~ 3.5
- Drift Velocity ($V_p$) ~ 2.0
- Saturation Velocity ($V_{sat}$) ~ 0.6
- GaAs
- Temperature ($T$) = 300 K

Figure 2.1: Schematic representation of the electron drift velocity vs electric field characteristic in GaAs at $T = 300$ K.
Figure 2.2: Schematic representation of the electron drift velocity vs electric field characteristic in GaN $T = 300$ K.
2.2 The Streaming Regime

In the “hot electron” regime, where the temperature of the carriers is higher than the semiconductor thermal bath, the electron distribution function is assumed to be an isotropic drifted Maxwellian distribution. This holds true if scattering in the semiconductor is dominated by quasi-elastic mechanisms where the energy of the scattered electron is little changed by the event.

If, on the other hand, inelastic mechanisms such as polar optical phonon emission scattering dominate, there is the possibility the distribution can become highly non-isotropic [43]-[45]. In this case, an electron will accelerate in the direction of an applied electric field until it reaches the polar optical phonon energy. If the electric field is not too strong, the electron will not have enough time to greatly exceed the phonon energy before a scattering event takes place. The electron will lose its energy almost entirely and return to the origin of the distribution plot. Again, the electron will drift in the direction of the field and the process will repeat itself indefinitely. Such motion will cause an anisotropic distribution (spindle shaped) in momentum along direction of the electric field and it will be nearly zero in the perpendicular direction (Fig. 2.3).

In real semiconductors, of course, electrons experience more than one type of scattering event. Acoustic phonons, impurities, dislocations, etc. will tend to spread the distribution over the entire momentum space. Additionally, inhomogeneous electric fields will accelerate the electrons above the polar optical phonon energy and they
Figure 2.3: Schematic representation a spindle shape distribution of electrons due to the streaming effect.
will subsequently return to a non-zero energy post scattering. If, however, the inelastic process dominates strongly enough, the carriers will undergo the cyclic motion described in the paragraph above, and will take on a highly anisotropic spindle shaped distribution.

2.3 Monte Carlo Model for Moderate Field III-nitrides

The so called Monte Carlo model for electrical device simulation, using random number generation to select carrier scattering events and final momentum states after scattering, provides a stochastic solution to the Boltzmann transport equation [38]. The main limitation of this method is that is it computationally intensive and the time required for simulation may be prohibitive for large-scale transient simulations. However, for steady state solutions it provides a intuitively satisfying physical description of carrier dynamics for bulk transport and device modeling. Although carrier transport in semiconductors is a large scale problem involving a vast number of carriers, it is possible to simplify the problem by tracing the motion of a single carrier in momentum space for a long period of time. If it is assumed that the carriers do not interact amongst themselves, a single carrier model provides a suitable approximation to the many-body problem.

The entire process, represented schematically in Fig. 2.4, can be summarized as
Figure 2.4: Schematic representation of the single particle Monte Carlo simulation.
follows. First the carrier is subjected to an electric field $E$ and its motion in the momentum space is followed for a constant time step. This motion is described semiclassically as

$$\Delta k = -\frac{eE}{\hbar} \Delta t$$ (2.1)

where $\Delta k$ is the incremental change in the electron wave vector during the time step $\Delta t$, $e$ is the electronic charge, and $\hbar$ is Plank’s constant divided by $2\pi$. The energy of the electron, as found from the parabolic approximation with the electron effective mass $m$, is used to calculate the scattering rates due to acoustic deformation and polar optical phonons, as well as ionized impurity scatterings. Three random numbers between 0 and 1 are then generated. The first random number $r_1$ is used to select an particular scattering mechanism from the normalized sum of the individual contributions. The second and third random number, $r_2$ and $r_3$, are used to select the azimuthal and polar angles of the final state wave vector $k'$. If the final pre-selected time for the simulation has not been reached, the process is repeated.

Electron scattering rates in the semiconductor, from the initial state $k$ to the final state $k'$, are calculated using Fermi’s golden rule

$$S(k, k') = \frac{2\pi}{\hbar} |\langle k' | H' | k \rangle|^2 \delta(\varepsilon_{k'} - \varepsilon_k - \Delta \varepsilon)$$ (2.2)

where $H'$ is the scattering Hamiltonian, $\Delta \varepsilon$ is the electron energy lost to the scattering event, and the $\delta$-function is used to maintain the conservation of energy. The scattering matrix element $|\langle k' | H' | k \rangle|$ must be evaluated for each scattering mecha-
Deviations in the periodic lattice potential due to vibrations propagating throughout the crystal may be quantized as phonons. The scattering rate due to this electron-phonon interaction is be calculated by choosing the appropriate interaction Hamiltonian, calculating the scattering matrix element, and applying Fermi’s golden rule.

Acoustic phonon modes are due to the displacement of neighboring crystal atoms in the same direction. In modeling acoustic phonons, it is assumed that the acoustic phonon energy $\hbar \omega$ is much less than $k_B T$ at room temperature, where $k_B$ is Boltzmann’s constant, and therefore assume the scattering is elastic. Additionally, the equipartition expression is used for the phonon population $n(\omega)$. In this approximation the acoustic phonon scattering rate is given as

$$\Gamma(\epsilon) = \frac{2\pi \Xi_d^2 k_B T}{\hbar c_L} \frac{2m^{3/2}}{\sqrt{\epsilon^2 A^2 \hbar^3}}$$

where $\Xi_d$ is the deformation potential constant and $c_L$ is the elastic constant of the material. It is seen that the acoustic phonon scattering rate has a strong dependence on temperature, a property which will be exploited later in this study.

Polar optical phonons in ionic crystals, due to longitudinal vibrations in the crystal lattice, are dominant in compound semiconductors such as GaAs and GaN. Emission rates tend to be several times to an order of magnitude larger than absorption rates and are much less dependent on temperature than acoustic phonon rates. For moderate electric fields at low temperatures it is expected that polar-optical phonons will
be the dominate energy relaxation mechanism. The polar-optical phonon scattering rate for a phonon with wave vector $q$ is given by

$$\Gamma(\epsilon) = \frac{e^2 \omega}{8\pi \epsilon_p \epsilon} \left[ n(\omega) + 1/2 \pm 1/2 \right] \ln\left( \frac{q_{min}}{q_{max}} \right)$$  \hspace{1cm} (2.4)$$

where $q_{min}$, $q_{max}$, and $n(\omega)$ are

$$q_{min} = k[1 - (1 \pm \frac{\hbar \omega}{\epsilon})^{1/2}], \quad q_{min} = k[1 + (1 \pm \frac{\hbar \omega}{\epsilon})^{1/2}], \quad n(\omega) = 1 + \frac{1}{\exp[\hbar \omega/k_B T] - 1}.$$ \hspace{1cm} (2.5)$$

$$1/\epsilon_p = 1/\epsilon_s - 1/\epsilon_s, \quad \epsilon_s$$ is the static dielectric constant of the material, $\epsilon_{\infty}$ is the dielectric constant at optical frequency range, and $\hbar \omega$ is the optical phonon energy.

Heavily doped semiconductors contain large densities of ionized impurities from which electrons will scatter. At very low electron energies impurity scattering will dominate, but at moderate to high electric fields for moderately high doping it will be a secondary mechanism in comparison to polar-optical scattering. The ionized impurity scattering rate in the Brooks-Herring approach is give by

$$\Gamma(\epsilon) = \frac{2\pi N_I Z^2 e^4 (2m)^{(3/2)} \sqrt{\epsilon}}{4\pi^2 \hbar^2} \frac{1}{q_d (4k^2 + q_d^2)}$$ \hspace{1cm} (2.7)$$

where $1/q_d$ is the Debye length, $N_I$ is the impurity density, and $Ze$ is charge on the impurity atom.

After an electron has scattered from its initial to final state it is necessary to specify the final state wave vector $k'$. Due to the isotopic nature of acoustic phonon scattering in the spherical approximation, this may be accomplished in a straightforward manner
by taking momentum conservation into account. The polar and azimuthal angles between $k$ and $k'$ can be specified by

$$\theta = \arccos(1 - 2r_2)$$  \hspace{1cm} (2.8)

and

$$\phi = \arccos(2\pi r_3).$$  \hspace{1cm} (2.9)

In the case of polar-optical and ionized impurity scattering the situation is slightly more complicated and it is necessary to determine the polar angle through analytical formulas describing the angular distribution of the final state. For polar-optical phonons

$$\cos(\theta) = \frac{1 + f - (1 + 2f)}{f}$$  \hspace{1cm} (2.10)

where

$$f = \frac{2\sqrt{E E'}}{(\sqrt{E} - \sqrt{E'})^2}$$  \hspace{1cm} (2.11)

and the azimuthal angle may be determined in the previous manner. For ionized impurity scattering

$$\cos(\theta) = 1 - \frac{2r_2}{1 + (1 - r_2)(\frac{2k}{q_0})^2},$$  \hspace{1cm} (2.12)

and the azimuthal angle may be determined in the previous manner.
2.4 Streaming in GaN

We begin with the review of the possible hot electron kinetic regimes. Let us consider the case when the lattice temperature $T$ is less than the optical phonon energy $\hbar \omega$, such that

$$\exp(-\hbar \omega / k_B T) \ll 1. \quad (2.13)$$

If this inequality is strong, one can neglect processes of absorption of optical phonons. For materials with strong electron-optical phonon interaction, electron motion inside the sphere of the momentum space, $|\mathbf{P}| < P_0 \equiv \sqrt{2m\hbar \omega}$, (the so-called passive region) [46] differs from motion in the active region, $|\mathbf{P}| > P_0$ (where $|\mathbf{P}|$ is the momentum and $m$ is the effective mass). Indeed, under the condition of Eq. 2.12 in the passive region, the electrons can be scattered by impurities, acoustic phonons, etc., but they do not interact with optical phonons. Conversely, in the active region they are predominantly scattered by emitting optical phonons. Let electrons in the passive region be characterized by the momentum relaxation time, $\tau_p$, and the energy relaxation time, $\tau_\epsilon$. Then, the hot electron effects hold in the electric fields

$$E > E_{H1} = k_B T/ eV_T \sqrt{\tau_p/\tau_\epsilon}, \quad (2.14)$$

where $V_T$ is the thermal velocity of the electrons. Typically, electron scattering in the passive region is quasielastic (the energy losses during scattering events are much less than the average energy of the electrons), i.e., $\tau_\epsilon \ll \tau_p$. The range of moderate electric fields $E$ is defined as the range of heating fields for which the hot electrons are
predominantly in the passive region. In a polar material, the electrons gain energy above $\hbar \omega$ at the fields of about [47]

$$E_0 = \epsilon m \omega (1/\kappa_\infty - 1/\kappa_0) / \hbar,$$  \hspace{1cm} (2.15)

where $\kappa_\infty$, $\kappa_0$ are high- and low- frequency permittivities of the material, respectively. Thus, the range of fields $E_{H1} \ll E \ll E_0/2$ will be analyzed. For this field range, the different regimes can be qualitatively classified as follows:

1. the hot electron regime with multiple scattering in the passive region and almost isotropic distribution function at $E_{H1} < E \ll E_{H2}$, where $E_{H2} = 2\hbar \omega / eV_0 \tau_p$ with $V_0 = \sqrt{2\hbar \omega / m}$

2. the streaming regime (almost collisionless in the passive region) with strongly anisotropic distribution at $E > E_{H2}$

3. as the field increases, the streaming regime is broken by electron penetration into the active region, the hot electrons spread over a wide region of the momentum space.

Remarkably, the first two regimes are characterized by distributions that are almost independent of the field. The first regime manifests itself in a linear portion of the current-voltage (I -V) characteristics (the so-called “second ohmic” portion). The second regime demonstrates [48] velocity $V_{dr} \approx V_0/2$. The third regime shows quasisaturation of the drift velocity and weakly depends on the field. In traditional
materials like GaAs, InSb, etc., the first hot electron regime is quite pronounced and was observed experimentally. Two other regimes are considerably masked by the nonparabolicity and intervalley transfer effects. In the nitrides, the strong electron-optical phonon interaction, large intervalley separation, and very large breakdown fields make realization of the second and third regimes possible.

The electron kinetics in the nitrides were analyzed by using the Monte Carlo method. The electron bands for InN, GaN, and AlN were considered in the isotropic and parabolic approximation with parameters given in [49]. Scattering by ionized impurities, acoustic phonons, and polar optical phonons were taken into consideration. Corresponding scattering rates as functions of the electron energy are presented in Fig. 2.5. The estimates of the characteristic fields $E_{H1}$, $E_{H2}$, $E_O$ are presented in Table 2.1.

As examples of calculations of the electron distribution functions, the contour plots of these functions are depicted for GaN at two values of the electric field in Fig. (2.6) and (2.7). Using the distribution functions, basic characteristics of the electron kinetics for three materials, InN, GaN, and AlN were found. To present these results, it is convenient to rescale these characteristics to the units associated with the electron-optical phonon interaction-$\hbar\omega$, $P_0$, $[V_O$ and $E_0$ (see Table 2.1). Shown in Figs. 2.8 (a) and 2.8 (b)] are the dimensionless characteristics, the average drift velocity, the average kinetic energy associated with electron motion transverse to the field and the mean-square deviation of the longitudinal component of the electron
Figure 2.5: Total scattering rates as functions of energy due to impurity scattering, polar optical phonon emission, and acoustic phonons at $T = 77K$ and $N_D = 10^{16} cm^{-3}$.
Table 2.1: Characteristic parameters of the nitrides where $\hbar\omega$ is the polar optical phonon energy, $E_g$ is the band structure energy gap, $E_{th}$ is the drift velocity-electric field threshold field, $v_p$ is the peak electron velocity, and $v_1$ is the high field electron saturation velocity.

<table>
<thead>
<tr>
<th>Material</th>
<th>$\hbar\omega$ (meV)</th>
<th>$E_g$ (ev)</th>
<th>$E_{th}$ (kV/cm)</th>
<th>$v_p$ ($10^7$ cm/sec)</th>
<th>$v_1$ ($10^7$ cm/sec)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GaN</td>
<td>91</td>
<td>3.2</td>
<td>220</td>
<td>2.8</td>
<td>2.0</td>
</tr>
<tr>
<td>InN</td>
<td>72</td>
<td>1.9</td>
<td>60</td>
<td>4.4</td>
<td>2.8</td>
</tr>
<tr>
<td>AlN</td>
<td>110</td>
<td>6.0</td>
<td>440</td>
<td>2.25</td>
<td>2.1</td>
</tr>
</tbody>
</table>
Figure 2.6: Momentum space distribution functions at $T = 77K$, $N_D = 10^{16} cm^{-3}$ and $E = 10 kV/cm$. Each contour line represents increase of 0.1 from 0.1 to 0.9.
Figure 2.7: Momentum space distribution functions at $T = 77K$, $N_D = 10^{16} cm^{-3}$ and $E = 60kV/cm$. Each contour line represents increase of 0.1 from 0.1 to 0.9.
Figure 2.8: (a) Moderate field drift velocity as a function of dimensionless field, (b) Longitudinal (solid line) and transverse (dotted line) components of the average electron kinetic energy as a function of dimensionless field. $T = 77K$ and $N_D = 10^{16} \text{cm}^{-3}$. 
velocity:

\[ V_{dr} = \frac{\langle V_i \rangle}{V_0}, \quad \epsilon_l = \frac{\langle V_i^2 \rangle}{V_0^2}, \quad \epsilon_t = \frac{\langle V_i^2 - V_{dr}^2 \rangle}{V_0^2}, \quad (2.16) \]

respectively. Here \( \langle \ldots \rangle \) means averaging over the distribution function, the indexes \( l \) and \( t \) indicate directions along and transverse to the field, respectively. The dimensionless field is \( \mathcal{E} = 2E/E_0 \).

According to Fig. 2.5, the rates of optical phonon emission are indeed much higher than other scattering rates. This supports the aforementioned difference of the passive and active momentum space regions. Then, the estimates presented in Table 2.1 show that the characteristic fields \( E_{H2} \) are of about several kV/cm \( (\mathcal{E}_{H2} \approx 0.01) \). At higher fields, when the criterion of Eq. 2.16 is met, the optical phonon emission processes start to control the kinetics. A kind of the streaming regime is formed: the spreading of the carriers over the “transverse” momenta decreases with the increase in \( \mathcal{E} \). This manifests itself in decreasing of the transverse average energy \( \epsilon_t \) as shown in Fig. 2.8 (b). The minimal values of \( \epsilon_t \) are close to the lattice temperature \( (\approx 77 \text{ K for InN}) \). As the drift velocities \( v_{dr} \) approach the high value \( \approx 1/2 \), as seen from Fig. 2.8 (a). The distribution function takes on the spindle shape as indicated by Fig. 2.6. Notice that almost all electrons have positive momentum component \( p_l \) and the penetration of the electrons into the active region is quite small. In this transient field range \( \mathcal{E} < 0.04 \), the dependences \( \epsilon_t(\mathcal{E}), \epsilon_l(\mathcal{E}), \) and \( v_{dr}(\mathcal{E}) \) are slightly different for the three nitrides. The electric fields corresponding to the lowest \( \epsilon_t \) and the maximal ratio \( \epsilon_l/\epsilon_t \) can be interpreted as optimal fields for the streaming regime (most close to
the ideal streaming). These fields are found to be 0.01, 0.04, and 0.02 for InN, GaN, and AlN, respectively.

As the electric field is increased further, the electron kinetics become entirely controlled by optical phonons (2. and 3. regimes). Under these regimes, the electron characteristics are *independent* of the material parameters in the herein introduced dimensionless representation. Figures 2.8 (a) and 3(b) clearly demonstrate this universal behavior: for a highfield range the results almost *coincide* for all studied nitrides. Most significantly, in a wide range of the electric field from $\mathcal{E} \approx 0.04$ to $\mathcal{E} \approx 0.3$, all characteristic parameters, $\epsilon_t$, $\epsilon_t$, and $v_{dr}$ are very slowly dependent on the field. Small variations in $\epsilon_t$ and $\epsilon_t$ indicate that the distribution function approximately preserves its shape. The drift velocity demonstrates a linear portion with small slope (almost quasisaturation). From these data, for this portion $\partial v_{dr} / \partial \mathcal{E}$, i.e., the differential mobilities are 290 cm$^2$/Vs, 84 cm$^2$/Vs, 18 cm$^2$/Vs for InN, GaN, and AlN, respectively were obtained. These values are considerably less than the values of the low-field mobilities estimated for the scattering rates of Fig. 2.5. At the end of this quasisaturation portion, both the penetration of the electrons into the active region and subsequent optical phonon emission destroy the spindle shape of the distribution. The shape of the electron distribution is depicted in in Fig. 2.7. Still, a dominant number of the electrons have positive longitudinal component of the momentum $p_l$.

At fields above $\mathcal{E} \approx 0.3$, the electron distribution spreads quickly over the momentum space, the electron energy sharply increases, as seen from Fig. 2.8 (b). The
system approaches the regime of the runaway of the electrons \[47\]. For the considered model of the electron spectra, the threshold electric field of the runaway effect in polar materials is \( E \approx 0.5 \ [50] \).

### 2.5 Conclusion

In conclusion, the problem of hot electrons in polar materials under moderate electric fields was considered. The analysis was applied to the group-III nitrides. Specifically, the distribution functions and field dependences of basic hot-electron characteristics were studied. It was established that optical phonon scattering becomes dominant in relatively low electric fields (the kV/cm range). As the result of this strongly inelastic scattering, the spindle-shaped electron distribution occurs. Formation of the streaming-like transport regime is supplemented by a nonmonotoneous dependence of the electron transverse energy \( \epsilon_t \). The regime manifests itself in an extended linear portion of the IV characteristic with very small differential mobility (almost saturation regime). It is proved an universal character of this behavior for all three nitrides (it is valid also for their alloys). The discussed regimes can be experimentally detected not only through the measurements of the IV characteristic, but also through the study of transverse hot electron effects. Specifically, the thermopower (Seebeck coefficient) of hot electrons measured in directions transverse to the current gives directly the transverse energy \( \epsilon_t \) (see \[51\] and references
Therein). The thermopower measurements would allow to find an optimal streaming regime. A spindle-shaped electron distribution is favorable for the practical application generation of microwave emission in sub-THz range (see also recent calculations of high-frequency differential mobility for GaN in [52]).

\footnote{This was, in part, published in Phys. Status Solidi B [53] and Appl. Phys. Lett. [69]}
Chapter 3

Extension of the Monte Carlo Method to Describe Bulk GaAs Electron Spin Dynamics

3.1 Introduction

Traditionally, only the charge of electrons has been utilized in the field of electronics and the quantum mechanical spin has been all but ignored. Recently however, there has been an increasing interest in the emerging field of spin electronics (spintronics), where the electron’s spin degree of freedom is exploited [55]- [57]. Many devices and applications, including giant-magnetoresistive structures (GMR) [58] and magnetic random access memories [59], have been suggested with varying degrees of
success. Furthermore, the suggestion of utilizing electron spin for quantum information processing is a natural extension of spintronics since the electron provides an ideal condition for a qubit.

The development of technology based on GMR, a phenomenon first reported in 1988 [60], has been the most commercially viable application to date. GMR occurs in a multi-layered structures composed of a non-ferromagnetic layer sandwiched between two ferromagnetic layers. The ferromagnetic layers naturally align themselves in an anti-parallel state. As electrons with mixed spin states pass through the structure they experience a large amount of scattering. In the presence of a magnetic field, the ferromagnetic layers are aligned in a parallel state and the population of electrons with parallel spins pass through with less scattering, leading to a decrease in the electrical resistance of the structure. The near ubiquitous application of GMR to hard drive sensing technology led to a dramatic increase of drive storage size and had an undeniable effect on the current state of computing [55].

The rapid success of GMR applications encouraged many areas of new research, including those attempting to use the charge and spin of electrons simultaneously. Of the potential applications, the hybrid devices [61] that combine ”traditional” semiconductor electronics with the utilization of the spin state are currently at the center of attention for their increased functionality and the ease of integration. Electron spin states in semiconductor structures relax (depolarize) by scattering with imperfections or elementary excitations such as other carriers and phonons. Therefore, to
realize any useful spintronic devices, it is essential to understand and have control over spin relaxation such that the information is not lost before a required operation is completed. So far, most of the studies on spin relaxation have been focused on electrons with a thermal or near-thermal distribution [62]. However, electron spins in the spin-based devices can be subject to highly non-thermal transport conditions including high drift fields for high-speed transfer of spin information.

The extension of the previous Monte Carlo method of simulation to include the description of electron spin provides a useful means by which to study spin depolarization in semiconductors. While the traditional Monte Carlo method only traces the evolution electron wave vector and real space position, it is possible to include spin evolution simultaneously and gain critical insight into the parameters which influence electron spin dynamics.

3.2 Simulation Method and Analysis

In this work, the influence of transport conditions on electron spin relaxation in n-type GaAs is investigated. A Monte Carlo approach is used to simulate electron transport, including the evolution of spin polarization, [63] to determine spin relaxation lengths and times. A non-parabolic energy-band model (with $\Gamma - L - X$ valleys) is used along with the relevant momentum relaxation mechanisms such as polar optical and acoustic phonon deformation potential scattering. Of the three main spin relax-
ation mechanisms [i.e., Bir-Aronov-Pikus, Elliot-Yafet, and D’yakonov-Perel’ (DP) mechanisms], [62, 64, 65] only the DP processes is considered since this is the dominant mechanism in the regime of interest, namely GaAs at 300K. It is also important to note that the current study is limited to the low energy cases, such that electrons are found only in the Γ valley. This is due to the lack of materials parameters on spin-orbit splitting in higher energy valleys.

The DP Hamiltonian due to spin-orbital splitting of the conduction band may be written as [66]

\[ H = \frac{\hbar}{2} \vec{\sigma} \vec{\Omega}_{\text{eff}}; \]  (3.1)

and

\[ \vec{\Omega}_{\text{eff}} = \frac{\alpha \hbar^2}{m \sqrt{2mE_g}} [k_x(k_y^2 - k_z^2)\hat{x} + \text{cyclic permutations}] ; \]  (3.2)

where \( \alpha \) is a dimensionless, material-specific parameter which gives the magnitude of the spin-orbit splitting \( \alpha \simeq 4\eta/\sqrt{3 - \eta} \frac{m}{m_0} \) and \( \eta = \Delta/(E_g + \Delta) \), \( m \) is the effective mass, \( \vec{k} \) is the electron wave vector, \( E_g \) is the energy separation between the conduction band and valence band at the Γ point, and \( \Delta \) is the spin orbit splitting of the valence band. The material parameters for GaAs are listed in Table 3.1.

The quantum mechanical description of the evolution of the spin 1/2 is equivalent to the evolution of the classical momentum \( \vec{S} \) under an effective magnetic field \( \vec{\Omega}_{\text{eff}} \) with the equation of motion
Table 3.1: Material Parameters for GaAs. $m/m_0$ is the Γ valley effective mass ratio, $\hbar\omega_0$ is the optical phonon energy, $E_l$ is the acoustic phonon deformation potential, $E_g$ is the energy band gap separation at the Γ point, $\alpha_{np}$ is the non-parabolicity factor in the Γ valley, and $\Delta$ is the spin-orbit splitting of the valence band.

<table>
<thead>
<tr>
<th>$m/m_0$</th>
<th>$\hbar\omega_0$</th>
<th>$E_l$</th>
<th>$E_g$</th>
<th>$\alpha_{np}$</th>
<th>$\Delta$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>eV</td>
<td>eV</td>
<td>eV</td>
<td>eV</td>
<td>eV</td>
</tr>
<tr>
<td>0.067</td>
<td>0.0354</td>
<td>7.0</td>
<td>1.424</td>
<td>0.616</td>
<td>0.341</td>
</tr>
</tbody>
</table>
\[
\frac{d\vec{S}}{dt} = \vec{\Omega}_{eff} \times \vec{S}.
\] (3.3)

Figure 3.1 depicts the average polarization \( \langle P \rangle \) of electrons calculated as a function of distance in GaAs. The simulation follows the evolution of \( 1 \times 10^4 \) spin-polarized electrons from an injection plane. Although all electrons are initially polarized \( \langle P_0 \rangle = 1 \), polarization at \( x = 0 \) in this figure is not exactly unity due to the averaging over a finite mesh size. Clearly, \( \langle P \rangle \) decays nearly exponentially with an order of magnitude drop (to 0.1) in approximately 4 \( \mu m \) to 7 \( \mu m \) (5.5 \( \mu m \) to 9 \( \mu m \) when the non-parabolicity is not considered).

The observed dependence of decay on the applied electric field is non-monotonous with the result of 2.5 \( kV/cm \) placed between the two cases with smaller fields. This can be explained by the two competing factors that contribute to the spin relaxation distance. As the field becomes larger in the linear regime, the electron momentum and the drift velocity increase in the direction of the field. On the other hand, the increased electron momentum also brings about a stronger effective magnetic field as shown in Eq. (3.2). Consequently, the electron precession frequency becomes higher, resulting in faster spin relaxation (i.e., shorter spin relaxation time). The interplay of these opposing trends (i.e., higher drift velocity and shorter relaxation time) determines the observed behavior of spin relaxation length as a function of electric field.

To examine the dependence of spin relaxation in detail, the spin relaxation rate \( \tau_s^{-1} \) is calculated as a function of electric field. The value of \( \tau_s \) is estimated by
Figure 3.1: Polarization $< P >$ of injected electrons as a function of distance.
approximating the spin decay to be exponentially dependent on length. The slope of Fig. 3.1 may be taken to be a characteristic length $L_D$, such that

$$< P > = A \exp \left(-\frac{L}{L_D}\right);$$

(3.4)

where $A$ is a normalization factor. The spin relaxation rate may then be computed as $\tau_s^{-1} = v_{dr}/L_D$, where $v_{dr}$ is the average drift velocity. For comparison, the results for the parabolic energy band are shown in Fig. 3.2 along with those with the non-parabolicity.

As expected, the spin relaxation rate increases rapidly with the applied electric field, which is also in accord with a recent experimental observation. [67] Although $\tau_s$ for low electric fields is nearly the same in both the parabolic and non-parabolic models, the spin relaxation rate becomes considerably larger in the non-parabolic case for fields higher than approx. 1.5 kV/cm. This is due to the growing significance of the non-parabolicity as the electron energy increases. The values for $\tau_s$ at the low fields agree well with those obtained for near thermal electrons. [65]

The dependence of spin relaxation on electric field can be best understood by considering the functional form of the effective magnetic field in Eq. (3.2). When the applied electric field is along the $x$ direction, the interaction Hamiltonian reduces approximately to

$$H \propto (k_z \hat{z} - k_y \hat{y})k_x^2.$$  
(3.5)
Figure 3.2: Spin relaxation rate $\tau^{-1}$ as a function of electric field $F$. The data points are the results calculated with or without the non-parabolicity. The solid line represents the $< k^2_x >$ scaling for the non-parabolic band.
Since the average values of $k_y$ and $k_z$ remain small, it is reasonable to assume that $\tau_s^{-1}$ will scale as $< k_x^2 >$. The solid line in Fig. 3.2 provides the $< k_x^2 >$ scaling for the non-parabolic case, which clearly illustrates good agreement over the entire field range under consideration. This finding indicates that the common assumption of electron temperature $T$ to the third power dependence \[ 1/\tau_{DP} \propto (k_B T)^3 \tau_p, \] where $\tau_p$ is the momentum relaxation time \[62, 65\] substantially overestimates the spin relaxation rates in the drift regime. Considering the nature of drift in this case, the $T^2$ scaling may be more appropriate although its applicability is also limited due to the non-parabolic energy band. Hence, calculation of $\tau_s^{-1}$ in the drift regime requires accurate description of electron distribution function.

In addition to the influence of the drift field, the spin transport and relaxation with varying injection energies is investigated. As mentioned earlier, one of the fundamental challenges in spintronics has been the electrical injection of spin polarized current into a semiconducting material. Noting recent suggestions \[68\] for the utilization of tunnel injection, relatively high electron energies at the injection point may be anticipated.

Plotted in Fig. 3.3 are the results of simulations where the injection energy and applied electric field are changed. It can be seen that the electrons quickly lose the extra energy and their momentum distribution stabilizes within $1 \mu m$ or so, even in the cases of higher energy injection (200 $meV$). Therefore, there are two distinct slopes. The first is a more rapid decay in the non-local transport region, corresponding to a
Figure 3.3: Electron polarization $< P >$ vs. distance as a function of injection energy and applied electric field.
large $\vec{k}$ and subsequently a large precession vector $\vec{\Omega}_{\text{eff}}$. Once thermalization occurs, the slope becomes smaller and eventually coincides with those shown in Fig. 3.1 with corresponding electric fields. For the 200 $meV$ case with an applied field of 1 $kV/cm$, the reduction in depolarization length is fairly significant, approximately 20 %.

### 3.3 Conclusion

In summary, spin-dependent transport in GaAs in the drift regime has been investigated. Specifically, the spin relaxation time and characteristic decay lengths based on a Monte Carlo model were calculated. The decay of electron spin polarization is found to be nearly exponential and the length at which spin relaxation/depolarization occurs was found to be relatively large, on the order of $5-10 \mu m$. It is also found that the spin relaxation depends strongly on the drift conditions, scaling as the square of the electron wavevector in the direction of the field. Hence, the commonly assumed $T^3$ scaling is not applicable in the drift regime. When the electrons are injected with a high-energy, a significant reduction is observed in the spin relaxation length. Our calculation results are in good agreement with the data available in the literature.

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1This was published, in part, in *Appl. Phys. Lett.* [69]
Chapter 4

Terahertz Generation in

Nitride-based Diodes

4.1 Transferred Electron and Gunn Effect

The Gunn effect, due to the negative differential resistance caused by the inter-valley transfer of hot electrons, is well known in bulklike two terminal devices [70]. The effect is characterized by the formation of an electron accumulation layer at one contact, that eventually develops into a stable space-charge domain [71]. This domain drifts in an electric field toward the opposite contact and is absorbed and registered as a signal upon exiting the channel. The main conditions of operation in such a device are that (i) the domain nucleates and fully forms before it can be absorbed and that (ii) the domain stabilizes, i.e. its relaxation rate due to intervalley transfer is slower
than the frequency of oscillation. The frequency of this mode is only dependent on the amount of time it takes the domain to nucleate, traverse the channel, and reach the opposite contact. The oscillation frequency may then be controlled by an external cavity and the applied bias voltage which determines the rate of drift of the domain.

This high field phenomenon is due to the accumulation of electrons near the cathode as a result of current injection. A nonuniformity in the charge density results in a highly inhomogeneous electric field distribution with some regions of the diode being in the NDR region of the electric field-drift velocity curve. Electrons in the regions where the local electric field is larger than the threshold field, $E_{th}$, will slow down, thus having a tendency to "bunch up", creating an even larger inhomogeneity in the electric field distribution. This process continues until a stable space-charge dipole is formed, that in time traverses the entire channel from cathode to anode where it is eventually absorbed. The frequency of operation is directly dependant on the length of the channel and the velocity at which the dipole drifts. Previously studies, which utilized Monte Carlo simulations and a lumped element approximation for a microwave resonator, have shown that upper frequency limitations for the Gunn mode in GaAs are on the order of a few hundred GHz [72].

The wide bandgap group III-nitride semiconductors have several advantages including a large bandgap, a high breakdown electric field, and a high electron drift velocity, which makes them promising materials of choice for high-frequency, high-temperature, and high-power device applications [27],[73],[74]. In addition to three-
terminal devices [27], various concepts for THz signal generation have been proposed and explored in simple two-terminal (diode) configurations based on the fundamental properties of high-field transport in the nitrides. These include optical phonon transit-time resonance emitters [75]-[77], impact Avalanche transit-time diodes [78, 79], as well as Gunn diodes utilizing various types of Gunn domain instabilities [80]-[84] or alternative modes of operation with suppressed Gunn domain formation [85, 86]. The latter represents the regime with limited space-charge accumulation (LSA) in the active region [87]. Under this regime, the space-charge will be totally relaxed as the ac field drops into the passive region of positive differential mobility and will be unable to propagate the entire length of the channel. A diode oscillator operating in the LSA mode may offer high output power with sufficient efficiency, effective space-charge control, and a short time of buildup of the quasistationary oscillations [88].

In comparison with GaAs-based structures, GaN active channels have the potential to achieve higher output powers at higher (THz) frequencies by taking advantage of larger electron velocities, reduced energy relaxation times, and the ability of the nitrides to sustain larger applied voltages and current densities. The electron mobility in GaN is lower than in GaAs. Therefore, the time for a stable domain to be built up is longer for the same given carrier (doping) density $n$ in the drift region $L_{ch}$ of the diode. As a consequence, the critical value imposed on the product $nL_{ch}$ for Gunn oscillations is also greater for GaN [$nL_{ch} > (5 - 8) \times 10^{12}\text{cm}^{-2}$ [80, 81]]. To achieve the highest frequencies and generation power simultaneously for structures with re-
duced channel length $L_{ch}$, the doping level is chosen to be much larger ($\simeq 10^{18}\text{cm}^{-3}$) than typically used for GaAs. Such doping densities correspond to large values of the $nL_{ch}$ product which varies approximately within $nL_{ch} = (2 - 3) \times 10^{13}\text{cm}^{-2}$ for different structures typically used in device simulations [80]-[83]. Electrical oscillations in GaN Gunn vertical diodes were reported in recent experiments [16] by using structures with $nL_{ch} = 5 \times 10^{13}\text{cm}^{-2}$ grown on $n$-GaN substrate and pulse bias regime to reduce self-heating.

To achieve stable generation, it is necessary to put the active diode into a resonant system. In this paper, a nonlinear analysis and simulation of the generation mode in a GaN submicrometer diode, coupled to an external resonant circuit, where the active region (doping and length) is chosen such that the $nL_{ch}$ product is close to (or less than) its characteristic critical value is provided. In this case, Gunn domain formation is expected to be suppressed and the operation regime may be close to the LSA mode. Specifically, a quantitative evaluation of the main performance parameters, output power, efficiency, and operating frequency, as well as higher-order harmonic contributions to the generated THz signal, is made. Also, the frequencies for which generation is possible are analyzed, depending on the load resistance and the bias voltage.
4.2 The Device Model and Calculation Method

4.2.1 Diode Equations

The oscillator diode is modeled as a one-dimensional bulk-like device using the drift-diffusion approximation for the high-field carrier transport in an $n^+nn^+$ structure. The contact regions are represented by heavily doped semiconductor regions, at each end of the active channel, of a length $L_c$ and a doping density much higher than that in the channel. The $n^+n$ and $nn^+$ interfaces are assumed to be abrupt junctions with a finite slope. Therefore, the description of our device consists of the continuity equation

$$\frac{\partial j(x,t)}{\partial x} + q \frac{\partial n(x,t)}{\partial t} = 0 \quad (4.1)$$

the Poisson equation

$$\frac{\partial E(x,t)}{\partial x} = \frac{q}{\epsilon}[n(x,t) - n_0(x)] \quad (4.2)$$

and the current density

$$j(x,t) = qnv_d - qD \frac{\partial n}{\partial x}. \quad (4.3)$$

Here, $n(x,t)$ is the carrier distribution, $n_0(x)$ is the doping density, $E(x,t) = -\partial \varphi(x,t)/\partial x$ is the electric field, $\varphi(x,t)$ is the electrostatic potential, $v_d(E)$ is the carrier drift velocity dependent on the local instantaneous electric field, $D$ is the diffusion coefficient (which is assumed to be a constant), $q$ is the electron charge, $x$ is the spatial variable, and $t$ is the time. The $x$ axis is oriented along the channel from source to drain.
We adopt an analytical approximation for the drift velocity-electric field characteristic (i.e., absolute value of $v_d$ vs. absolute value of $E$), developed by a least squares fit to the results of a Monte Carlo calculation [89]

$$v_d(E) = \frac{\mu_0 E + v_1 (\frac{E}{E_1})^\alpha}{1 + (\frac{E}{E_1})^\alpha + \zeta (\frac{E}{E_1})^\beta} \quad (4.4)$$

where $v_1$ is the saturation velocity, and $E_1, \alpha, \beta, \text{ and } \zeta$ are fitting parameters. It should be noted that there is a fair amount of variance in the literature concerning the exact shape of the curve for both experimental measurements [90]-[96] and theoretical calculations [97]-[104]. In particular, values for peak velocity, $v_p$, and threshold field, $E_{th}$, are varied with a range of approximately $(2-3) \times 10^7 \text{ cm/s}$ and $(150-220) \text{ kV/cm}$, respectively, depending on the conditions of simulations and measurements. The calculated $v_d(E)$ curve used in the simulations corresponds to the low-field mobility $\mu_0 = 990 \text{ cm}^2/\text{V-s}$, $v_1 = 1.9 \times 10^7 \text{ cm/s}$, and the specific numbers for the fitting parameters in (4.4) obtained from a regression analysis to fit the curve to the results of a Monte Carlo simulation for electron transport in bulk wurtzite GaN ($n_0 = 1 \times 10^{17} \text{ cm}^{-3}$, $T_0 = 300 \text{ K}$) [89]; the threshold field $E_{th} = 220 \text{ kV/cm}$, the peak drift velocity $v_p = 2.8 \times 10^7 \text{ cm/s}$, and the ratio $v_p/v_1 = 1.5$.

The boundary conditions for the $n^+nn^+$ structure are imposed through the electrostatic potential and electron density as follows

$$\varphi(0, t) = V_d(t), \quad \varphi(L_d, t) = 0$$
and

\[ n(0, t) = n_0(0), \quad n(L_d, t) = n_0(L_d) \]  \hspace{1cm} (4.5)

\((t > 0)\), where \(L_d = L_{ch} + 2L_c\) is the diode length. Then it follows from (4.2) and (4.5) that \((\partial E(x, t)/\partial x)|_{0,L_d} = 0\) at the boundaries \(x = 0\) (cathode) and \(x = L_d\) (anode).

The initial distributions at \(t = 0\) of the potential (field) and carrier density are taken to be the thermal-equilibrium values at zero bias.

For the numerical integration of the set of space-dependent and time-dependent equations (4.1)-(4.5), a procedure similar to that described in [88] is used. From the Poisson equation we can write

\[ \frac{\partial n(x, t)}{\partial t} = \frac{\varepsilon}{q} \frac{\partial^2 E(x, t)}{\partial x \partial t} . \]  \hspace{1cm} (4.6)

Substitution into the continuity equation gives, after integrating it over \(x\), the total current density through the diode

\[ J_d(t) = j(x, t) + \varepsilon \frac{\partial E(x, t)}{\partial t} \]  \hspace{1cm} (4.7)

which is a function of time \(t\) only. Here, the first term on the right-hand side is the conduction current density (4.3) and the second term is the displacement current density. Then by eliminating \(n(x, t)\) from (4.2), (4.3) and (4.7), we obtain

\[ \frac{\partial E}{\partial t} = D \frac{\partial^2 E}{\partial x^2} - v_d(E) \frac{\partial E}{\partial x} + \frac{q}{\varepsilon} \left\{ \frac{1}{q} J_d(t) - v_d(E)n_0 + \frac{D}{dx} \right\} . \]  \hspace{1cm} (4.8)

Equation (4.8), supplemented with boundary conditions and the initial condition \(E(x, 0) = E_i(x)\), determines the spatial-temporal variation of the electric field in the
diode. For a given electric field $E(x,t)$, the carrier density distribution is calculated from the Poisson equation

$$n(x,t) = n_0(x) + \frac{\varepsilon}{q} \frac{\partial E(x,t)}{\partial x}.$$  \hspace{1cm} (4.9)

The total current density, given in (4.7), can be represented as a sum of the electronic and capacitive current density

$$J_d(t) = J_e(t) + J_c(t)$$  \hspace{1cm} (4.10)

where

$$J_e(t) = \frac{1}{L_d} \int_0^{L_d} (qn v_d - qD \frac{\partial n}{\partial x}) dx$$  \hspace{1cm} (4.11)

and

$$J_c(t) = \frac{1}{L_d} \int_0^{L_d} \varepsilon \frac{\partial E}{\partial t} dx = \frac{\varepsilon}{L_d} \frac{dV_d}{dt}.$$  \hspace{1cm} (4.12)

This allows the capacitive current term of the diode to be represented by a parallel capacitance within the external circuit. The voltage across the diode $V_d(t)$ must be equal to the integral of the electric field inside the device

$$V_d(t) = \int_0^{L_d} E(x,t) dx.$$  \hspace{1cm} (4.13)

This provides the important connection between the equations describing the external circuit and those describing the carrier dynamics inside the diode.
4.2.2 Circuit Equations

In the simulation, we use a parallel RLC resonant circuit (Fig. 4.1) to excite oscillations, which establishes a quasi-sinusoidal voltage across the diode. The equations of the oscillator circuit may be determined by Kirchhoff’s method and are found to be

\[ I(t) = C \frac{dV_d(t)}{dt} + I_e(t) \]  \hspace{1cm} (4.14)

and

\[ \frac{dI(t)}{dt} = -\frac{1}{R_L} \frac{dV_d(t)}{dt} - \frac{V_d(t) - V_b}{L} \]  \hspace{1cm} (4.15)

where \( I(t) \) is the total current in the resonant circuit, \( I_e(t) = SJ_e \) is the electronic current through the diode, \( S \) is the diode cross-sectional area, \( V_b \) is the battery voltage, \( L \) is the inductance, and \( R_L \) is the load resistance. The total capacitance \( C = C_c + C_d \) contains both the circuit capacitance \( C_c \) and the diode capacitance \( C_d = \varepsilon S / d \). The initial conditions to (4.16) and (4.17), which determine two variables \( V_d(t) \) and \( I(t) \), can be written as \( V_d(0) = V_b \) and \( I(0) = \text{const} \). The circuit equations are coupled with the diode equations through the diode current \( I_d(t) = SJ_d(t) \) and voltage \( V_d(t) \).

The equations of the oscillator circuit may be rewritten in the form

\[ \frac{dV}{dt} = \frac{1}{C} I - \frac{1}{C} I_e \equiv P(V, I) , \]  \hspace{1cm} (4.16)

and

\[ \frac{dI}{dt} = \frac{1}{R_L C} I_e - \frac{1}{R_L C} I - \frac{1}{L} V \equiv Q(V, I) . \]  \hspace{1cm} (4.17)
Figure 4.1: The parallel RLC circuit used in the device simulation.
Here, $V(t) = V_d(t) - V_b$ The initial conditions can be written as $V_d(0) = V_b$ and $I(0) = \text{const}$, where $V_b$ is the external applied bias voltage.

For the local quasi-steady-state approach used in the simulation, the electronic current $I_e$ can be considered as a function of diode voltage $V_d$, $I_e = I_e(V_d)$. This allows one to analyze the possible time-dependent solutions of Eqs. (4.16), (4.17) on the phase plane $(V, I)$ for different values of the parameters $C, R_L, L$, and $V_b$. The singular points, determined by the equations $P(V, I) = 0$ and $Q(V, I) = 0$, correspond to the steady-state solutions, $V_d = V_b$ and $I = I_e$. The generation threshold can be found from a linear analysis to be $P(V, I) = aV + bI$, $Q(V, I) = cV + dI$ by assuming only small deviations of the variables $V$ and $I$ around the singular points. The coefficients are found to be $a = -G_d/C$, $b = 1/C$, $c = (G_d/R_L C)/L$ and $d = -1/R_L C$, where $G_d = dI_e/dV = qn_0\mu_d S/L_d$ is the differential diode conductance.

Making use of the general methods for the investigation of singular points, [105] we find a focus for $4R^2C/L > 1$ and a node for $4R^2C/L < 1$, where $R = R_L R_d/(R_L + R_d)$ and $R_d = 1/G_d$ is the differential resistance. The singular point is stable (i.e., stable focus or node) for $G_d + 1/R_L > 0$ and unstable for the opposite inequality $G_d + 1/R_L < 0$. The instability criterion given by the latter inequality determines the necessary conditions for generation, i.e., the generation threshold. In terms of the differential mobility, it may be expressed as $-\mu_d > (L_d/S qn_0 R_L)$. The phase trajectories associated with an unstable singular point describe transient oscillations followed by steady-state generation once they have approached the closed trajectory,
i.e., limit cycle. We note that the existence of a limit cycle for the considered oscillator follows from the well-known Bendixson criterion, [105] which establishes that the expression $F_B \equiv (\partial P/\partial V) + (\partial Q/\partial I)$ must change its sign in the relevant region of the phase plane. Then using $P(V, I)$ and $Q(V, I)$ given in Eqs. (4.16) and (4.17), we obtain $F_B = -(G_d + 1/R_L)/C$. It is seen that the condition for $F_B$ to change its sign coincides with the instability criterion mentioned above.

The diode and circuit equations are transformed into explicit finite difference equations and solved for each time step $\Delta t$ in the simulation. The spatial derivatives are approximated by a central, finite difference scheme. For the time derivatives, we use a backward finite difference approximation to update the voltage and current at the next time moment $t + \Delta t$ based on values at a previous time moment $t$. Care must be taken in choosing the length $\Delta x$ and time step $\Delta t$ of the spatial and time meshes so that the system algorithm is stable and the simulation does not diverge [106]. Using the initial conditions at the time moment $t = 0$, the values at the next time moment are calculated for a new field profile [Eq. (4.8)] and for the voltage $V_d(t)$ and current $I(t)$ [Eqs. (4.16) and (4.17)]. In each time step the field distribution $E(x, t)$ calculated from (4.8) is corrected by verifying the result of (4.13). An important consideration in determining the external circuit parameters is to ascertain the proper loading resistance of the resonant circuit. In order for stationary oscillations to be achieved, after some initial transient buildup, the negative differential resistance of the device must be equal to the load resistance of the circuit [107].
4.3 Calculation Results and Discussion

First the aspects establishment of steady-state oscillations in a very short diode are considered. In order to prevent Gunn domain formation the restriction that the product $nL_d < 3\varepsilon v_d/(q|\mu_d|)$ must be imposed, where $n$ is the carrier density, $L_d$ is the channel length, $\mu_d = dv_d/dE$ is the differential mobility, $q$ is the carrier charge, and $\varepsilon$ is the dielectric constant. For bulklike GaN, this gives $nL_d < 5.2 \times 10^{12} \text{ cm}^{-2}$, [85] which can be readily satisfied with a relatively low carrier density and short channel length; e.g., $n = 1 \times 10^{17} \text{ cm}^{-3}$ and $L_d = 100 \text{ nm}$ as used in the current calculation. The doping density $n_0$ is assumed to be uniform in the conducting channel and the diffusion coefficient $D$ to be a constant (a commonly accepted value of $D = 25 \text{ cm}^2/\text{s}$ was used for this numerical calculation). To determine the spatial-temporal variation of the electric field in the diode channel, it is assumed the boundary conditions are $E(0,t) = 0$, $E(L_d,t) = 0$ ($t > 0$). This corresponds to ohmic contacts in the context of a simplified theory which allows us to ignore the role of the contact regions[108] and the initial condition $E(x,0) = E_i(x)$.

The establishment of steady-state oscillations are demonstrated in Figs. 4.2 and 4.3 where the dynamic current-voltage characteristics calculated for two frequencies, 0.5 THz and 2.2 THz respectively, are shown. Two different transients can be distinguished in the figures. The initial (non-oscillating) part of the dynamic $I - V$ curves is due to an increase of the bias voltage which was ramped up linearly over
Figure 4.2: Dynamical $I(t) - V(t)$ characteristics for oscillation frequency $f = 0.5$ THz. The circuit parameters used were $R_L = 22.5 \Omega$, $L = 0.75$ pH, $C = 0.2$ pF (a) and $C = 2.4$ fF (b), and the bias voltage $V_b = 3.0$ V.
Figure 4.3: Dynamical $I(t) - V(t)$ characteristics for oscillation frequency $f = 2.2$ THz. The circuit parameters used were $R_L = 22.5 \ \Omega$, $L = 0.75 \ \text{pH}$, $C = 0.2 \ \text{pF}$ (a) and $C = 2.4 \ \text{fF}$ (b), and the bias voltage $V_b = 3.0 \ \text{V}$.
1 ps to prevent overshoot. This is followed by an initial oscillating transient leading to stationary oscillations of the diode voltage and current when the corresponding phase trajectory reaches the limit cycle. The entire cycle of operation over one period was examined and the electric field and charge dynamics inside the diode were analyzed in detail. Since the electric field is assumed to be identical at both (contact) boundaries, it follows from the Poisson equation that the total charge in the channel is zero and only its spatial distribution is time varying. This is analogous to a dipole oscillating between the anode and cathode. The diode voltage and current waveforms are dependent on the circuit parameters and are therefore dependent on the generation frequency. It can be seen that in the lower frequency limit of the LSA mode the voltage is strongly sinusoidal. Conversely, in the upper frequency limit it is less strongly sinusoidal owing to higher harmonic contributions.

For the $n^{+}nn^{+}$ structure, the channel length, channel doping density, contact length, and contact doping density are set to be $L_{ch} = 0.5 \, \mu m$, $n_0 = 1 \times 10^{17} cm^{-3}$, $L_c = 0.1 \, \mu m$, $n_0 = 1 \times 10^{19} cm^{-3}$, respectively. The doping density is assumed to be uniform in both the conducting channel and contact regions. To avoid numerical instabilities in the calculation procedure, the junctions are spread over a narrow interval near each interface. The cross-sectional area of the diode $S$ is taken to be $2500 \, \mu m^2$. The diode voltage and current are analyzed as functions of time for different values of the circuit parameters and bias voltage $V_b$ (The battery voltage is ramped up linearly over 1 ps to minimize overshoot). The transient characteristics of
the active diode exhibit the buildup of the diode voltage from \( t = 0 \) until a stationary oscillating state is achieved, typically over several oscillations. Depending on the circuit parameters and matching conditions the device may experience a short period of overshoot before a stationary state is fully realized. This is evident in Fig. 4.4, where after the voltage is ramped to \( V_b \), a transitory period exists before the voltage settles into stationary oscillations.

To avoid possible Joule heating of the diode, it is necessary to use a pulsed regime of operation with short pulses of about 1 ns and a duty cycle of 30-50 ns. A demonstration of stable negative differential resistance and electrical oscillations was recently reported [16]. This was obtained by the pulsed biasing of a vertical Gunn diode, with a channel doping of \( 1 \times 10^{17} \text{ cm}^{-3} \), grown on \( n \)-GaN substrate.

The shape of the voltage and electronic current waveforms, shown in Fig. 4.5, are inherently dependent on the external circuit parameters and therefore the frequency of oscillation. The analysis shows that for a diode operating near the lower frequency limit, the voltage is strongly sinusoidal. On the other hand, the electronic current clearly exhibits upper harmonic components. If a 90 degree phase shift is not maintained between the current and voltage waveforms, this may lead to the diode operating in a dissipative mode. Specifically, as \( V_d \) decreases towards its minimum value, the current can change from increasing to decreasing. When the electronic current is decreasing (increasing) concurrently with \( V_d \), the diode is temporarily functioning as a dissipative bulk resistor. As will be seen below, this leads to greater
Figure 4.4: Diode voltage as a function of time. The transient characteristics exhibit the buildup of the diode voltage from $t = 0$ until a stationary oscillating state is achieved.
Figure 4.5: Diode voltage (dashed) and electronic current (solid) vs. time for a diode with an oscillation frequency of 0.5 THz.
inefficiency in the diode operation. For a diode operating near the upper frequency limit, the voltage is less strongly sinusoidal. However, the electronic current in this case remains out of phase with $V_d$ for a greater portion of the period which leads to a greater dc-to-RF conversion efficiency.

Again, a diode model where the contact regions are represented by mathematical boundary conditions ($L_c = 0$) for Eq. (4.8) and are approximated by zero electric fields at the channel boundaries, $E(0, t) = 0$ and $E(L_{ch}, t) = 0$ is considered. These conditions correspond to ohmic contacts in the context of a simplified theory ignoring the role of the contact regions at the channel boundaries. Examining the entire cycle of operation over one period, the electric field inside the channel is plotted as a function of $x$ in Fig. 4.6 in evenly distributed time steps in the oscillation cycle. The diode voltage $V_d$ at each time step is shown in the inset. When the diode voltage $V_d$ is at its minimum value (point A in the inset), the field is almost homogenous in the majority of the diode. At point B the voltage begins to increase and the field starts to redistribute becoming more inhomogeneous. The voltage reaches its maximum near D, at which point the average electric field $E_{av}(t) = \frac{1}{L_d} \int_0^{L_d} E(x, t)dx = V_d(t)/L_d$ also reaches its maximum. This increasing inhomogeneity coincides with the growth of the accumulation layer near the cathode which begins to drift towards the anode. Of critical importance is that the electric field increases sharply in the direction of traveling accumulation layer. Although a Gunn domain does not form, the accumulation layer completely traverses the channel. Its spatial center corresponds
Figure 4.6: Electric field distributions for a diode without $n^+$ regions sampled throughout one period of oscillation. The inset shows the diode voltage vs. time over one period. Letters A to G correspond to samples taken at the times indicated on the inset.
to the moving peak of the electric field for which the value is never below $E_{th}$ long enough to completely destroy the accumulated charge. During the next cycle the voltage again begins to rise and the process is repeated. Similarly, the electric field and carrier density distributions are calculated at different instants of time for the $n^+nn^+$ structure described above and are shown in Figs. 4.7 and 4.8. With the addition of the contact regions, the electric field becomes less homogeneous in comparison with that shown in Fig. 4.6. This is due to the influence of the high-low junction interfaces, especially near the anode where a pronounced junction depletion layer is formed under the high bias conditions. However, the results show that the dynamics of the space-charge formation remains the same [Fig. 4.8], i.e., the accumulation layer is formed in the channel (curve B-C), moves towards (curves D) and reaches the anode (curves E-F) during one period of oscillation. Although the voltage is near its minimum at point A, there is still a finite amount of charge near the anode and the accumulation layer has not been fully quenched.

A Fourier series analysis is performed to examine the harmonic components of the diode voltage and electronic current and to facilitate the calculation of the generated power and dc-to-RF conversion efficiency. The average power across the device may be written as the integral of the instantaneous power over one period, $T$,

$$P_{av} = \frac{1}{T} \int_0^T V_d(t)I_e(t)dt ,$$

(4.18)

where the voltage and current are expended into the Fourier series. Carrying out
Figure 4.7: Electric field distribution for a $n^+nn^+$ diode with an oscillating frequency of 0.5 THz sampled throughout one period of oscillation similar to that shown in Fig. 4.6.
Figure 4.8: Electron density distribution for a $n^+nn^+$ diode with an oscillating frequency of 0.5 THz sampled throughout one period of oscillation similar to that shown in Fig. 4.7.
the integration, all the cross terms go to zero and only terms containing the same 
harmonic number of the voltage and current remain. The zeroth terms represent 
the dc components whereas the next terms correspond to the higher harmonics of 
the waveforms. The discrete Fourier transform [109] may be used to find an approx-
imation for the Fourier coefficients of the functions $V_d(t)$ and $I_e(t)$ obtained from 
the device simulation results. Calculation of the components of the diode voltage 
and electronic current spectra for a frequency of 0.5 THz, up to the 4-th harmonic, 
have shown that although there are significant contributions from upper harmonics, 
their phases are such that they do not overwhelm the fundamental. In addition, the 
frequency spectrum of the current exhibits a much smaller contribution of the funda-
mental harmonic, relative to the dc value, in comparison with the voltage frequency 
spectrum. When operating at lower frequencies, the fundamental harmonic is spread 
into the higher harmonics which is seen clearly in the nonsinusoidal nature of current 
waveform for those frequencies.

Utilizing the discrete Fourier transform, the average power (4.18) of the device 
can then be calculated as

$$P_{av} = P_{dc} + \sum_{n=1}^{\infty} P_{ac}^n$$  \hspace{1cm} (4.19)

where the first term of $P_{av}$ corresponds to the dc component of the power while the 
$n$-th term within the summation corresponds to the $n$-th harmonic of the ac power of 
the device. The average power may now be used to calculate the dc-to-RF conversion 
efficiency, $\eta$, given by $\eta = -P_{ac}/P_{dc}$. In Figs. 4.9 and 4.10, the generated power
Figure 4.9: Generated power as a function of load resistance, $R_L$, and frequency of operation.
Figure 4.10: The dc-to-RF conversion efficiency as a function of load resistance, $R_L$, and frequency of operation.
and conversion efficiency are shown as functions of frequency and of the circuit load resistance \( R_L \). It is seen that as the frequency is increased from the lower end of the generation spectrum, both the ac power and the conversion efficiency increase. This is in agreement with the previous analysis of the current and voltage waveforms for different frequencies, i.e., the current and voltage are closer to being 90 degrees out of phase over the entire period. Therefore, the device will be more efficient at higher frequencies with a maximum generated power of about 1 W and a dc-to-RF conversion efficiency of nearly 0.5 percent at a frequency of 0.5 THz \((R_L = 10 \text{ Ohm})\).

It can be noted that an ac power of about 100 mW is generated at a frequency of 0.65 THz. As the frequency is raised further, and the conditions for generation can no longer be satisfied, the output power will show a marked and abrupt decrease.

Preliminary simulations for a channel doping density of \( 5 \times 10^{17} \text{ cm}^{-3} \) are shown in Fig. 4.11. Increasing the doping density to slightly above the estimated critical value does not yet induce Gunn domain formation, though the qualitative criterion for the product \( nL_{ch} \) is weakly exceeded. Since the rate of the formation of the accumulation layers is also increased, due to the larger doping sen The maximum output power and conversion efficiency are now above 6 W and 1 %, respectively. Perhaps more importantly, the power and efficiency are greater than 1 W and 0.2 % at a frequency of 0.9 THz.

In the analysis, it is assumed that the kinetic coefficients depend on the instantaneous local electric field. This assumption is justified for small variations of the
Figure 4.11: Generated power (solid) and dc-to-RF conversion efficiency (dashed) vs. frequency for doping densities of $1 \times 10^{17} \text{ cm}^{-3}$ (1) and $5 \times 10^{17} \text{ cm}^{-3}$ (2).
electron density and electric field in the time and length scales of the energy relaxation
time $\tau_\varepsilon$ and the mean free path $l_\varepsilon$, respectively. For nitride-based structures, polar
optical phonon scattering is the dominant electron-phonon interaction and is the
largest contributor to the energy relaxation time at elevated (room) temperature,
which is estimated to be in sub-pico-second range $\tau_\varepsilon = (0.1-0.01) \text{ ps}$ $[l_\varepsilon = (10^{-2} - 10^{-3}) \mu\text{m} \ll L_{ch}]$ for GaN [110]. Hence, the upper frequency limit of interest can be
extended to the THz frequency range.

4.4 Conclusion

An efficient, compact, solid-state source of THz radiation with a sufficient power
output is currently unavailable. Therefore, the operation of a submicron GaN diode
in the THz regime was investigated by a large signal computer simulation. Carrier
transport in the device was treated by the drift-diffusion model, which included an
analytical approximation for the drift velocity-electric field curve, enabling the expeditious numerical calculation over a wide range of parameters. A Fourier analysis
was then employed to examine the resultant current and voltage signals. For a device
with a relatively lightly doped active channel ($1 \times 10^{17} \text{ cm}^{-3}$), operating in a regime
absent Gunn domain formation, is found to generate a large output power of $P_{ac} \simeq
1 \text{ W}$ with a dc-to-RF conversion efficiency of about half a percent.

\textsuperscript{1}This work to be published, in part, in J. Appl. Phys. [111] and IEEE Sensors J. [112]
Chapter 5

Electrothermal Simulation of a Terahertz Frequency Submicron GaN $n^+nn^+$ Diode Operating in the Pulsed Mode Regime

5.1 Introduction

In devices with high current densities and/or large electric fields, proper thermal management is critical to design [113]-[118]. The analysis in the previous chapter shows that decreasing the channel length $L_{ch}$ to achieve the highest possible frequency causes the electric field distribution in an $n^+nn^+$ diode to become strongly
inhomogeneous, especially in a narrow region near the anode. Under a high dc bias, the local electric field $E$ can reach a very high peak value ($\lesssim 10^3$ kV/cm) which corresponds to a high dissipated power of more than a hundred watts in the anode region. As a consequence, the local temperature increase due to Joule heating may become comparable to the initial (ambient) temperature after just a few nanoseconds of operation. Such a large production of heat during the early stages of generation process will result in a considerable degradation of the output diode performance, the ac power and efficiency, and may even result in the complete quenching of generation itself.

In the present study, self-consistent electrothermal simulations and an analysis of pulsed regimes of THz generation in a n-GaN NDR diode is performed. The diode is operated in a resonant circuit and self-heating effects due to dissipated Joule power in the conducting channel are included. Specifically, a quantitative evaluation of the parameters of operation including dc-to-RF conversion efficiency, ac generated power, temperature distribution and operating frequency is provided. To the best of the authors knowledge, there are no self-consistent electrothermal numerical simulations for such a device which include a detailed analysis of generated output power, conversion efficiency, and frequency of operation [119].

The drift-diffusion approximation to model the one-dimensional high-field electron transport in the vertical GaN-based $n^+nn^+$ bulk-like structure (Fig. 5.1) is used. The n-type channel is sandwiched between two heavily doped $n^+$ contact regions with
Figure 5.1: Geometry of the $n^+nn^+$ diode and substrate.
densities more than one order of magnitude greater than the channel. Electron transport in the diode is completely specified by Poisson’s equation, the current density and continuity equations, and the appropriate boundary conditions (BCs). A parallel RLC circuit was used to establish quasi-sinusoidal oscillations across the device. The equations for the circuit, determined by Kirchoff’s method, are coupled to the transport equations through the diode current. This system of equations, with the addition of the circuit initial conditions, completely describes the generation of ac power due to the exploitation of NDR in the electron drift-velocity field characteristic. Previous calculations utilizing this scheme for a submicron $n$-GaN diode, without the inclusion of self-heating effects, predicted high output powers in the THz frequency range [112].

5.2 Model and Analysis

To investigate heat transport within the diode channel and from the channel into the substrate, the time-dependent temperature distribution $T(x,t)$ in the device is found from the nonlinear heat conduction equation

$$c\rho \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}(k \frac{\partial T}{\partial x}) + g(x,t), \quad (5.1)$$

where $c$ is specific heat, $\rho$ is mass density, $k$ is thermal conductivity. The heat-generating region in the diode is described by the local heat source $g(x,t)$ determined by the instantaneous local (Joule) power $g(x,t) = j(t)E(x,t)$ dissipated in the diode channel, where $j(t)$ is the time-dependent current density. For the initial and BCs to
Eq. (5.1), a homogeneous temperature distribution given by the ambient temperature $T(x, t = 0) = T_0 = 300$ K, which is also maintained at the bottom of substrate $T(x, t > 0) = T_0$, for all time $t$ is assumed. It is assumed that there is zero heat flux through the rest of boundaries, i.e., side surface and top contact (adiabatic BCs). At the interface between the diode and substrate $x = 2L_c + L_{ch}$, the heat flux $q(x, t) = -k(T)(\partial T/\partial x)$ and temperature $T(x, t)$ are assumed to be continuous functions of the spatial coordinate $x$.

Shown in Fig. 5.2, is the dependence of the electron drift-velocity field characteristic on temperature, within the range from 300 K to 600 K, which was determined using an interpolation scheme utilizing coefficients obtained by fitting analytical approximations to data from Monte Carlo calculations [98]. The temperature dependence of the thermal conductivity $k(T)$ has been taken into account in the considered range of temperatures $k(T) = k_{300}(300/T)^\alpha$, where $k_{300} = 130$ Wm$^{-1}$K$^{-1}$ for GaN, 350 Wm$^{-1}$K$^{-1}$ for SiC, and the specific values of $\alpha$ have been taken from Ref. [120]. The entire program flow of the entire electrothermal simulation is shown schematically in Fig. 5.3.

Estimations show that the characteristic time scale of the thermal transport $\tau_{th}$ is of the order of ns and the characteristic time for electrical oscillations $\tau_e \simeq f^{-1}$ of the order of ps, where $f$ is the frequency. Due to the large aspect ratio $\tau_{th}/\tau_e \gg 1$ the instantaneous heat generation term in Eq. (5.1) can be replaced by the time average over one period of oscillation. For the numerical simulation to be self-consistent, the
Figure 5.2: Temperature dependent electron drift velocity vs. electric field used in calculation.
Calculate $V_{dr}$ for new $T(x)$

$V_{dr}(T=300\, K)$

Electrical Simulation
$E(x)$, $I(t)$, $V(t)$

Thermal Simulation
$T(x)$

Is $T(x) > 600\, K$ at any point in the channel?

No

Yes

EXIT

Figure 5.3: Schematic representation of the electrothermal simulation flow.
temperature dependence of the electron drift velocity should be taken into account. An explicit finite difference representation is found for the diode and circuit equations and is solved for time step $\Delta t_e$. A finite difference solution of $T(x, t)$ for the diode and substrate is then found from Eq. (5.1) using the time step $\Delta t_{th}$ for which the heat generation term is time averaged in the electronic time scale $\tau_e$. An electrical solution is then found for the updated temperature distribution and drift velocity across the diode and this procedure is iterated for the entire “on” state pulse width.

Examining the entire cycle of operation over one period, the electric field inside the channel is investigated as a function of $x$. In Fig. 5.4, the electric field distribution for different time moments in the oscillation cycle for an applied voltage $V_a = 13$ V is shown. The field is inhomogeneous and sharply peaked near the anode over the entire cycle. Since $j(t)$ is spatially independent, the Joule heating will be strongly localized in the region near the anode resulting in the asymmetric generation of heat. For this reason, it is necessary to orient the diode such that the high temperature region is adjacent to the ambient thermal reservoir providing a good thermal contact (Fig. 5.1).

The time-dependent temperature distribution in the GaN diode with a 1 $\mu$m thick SiC substrate is shown for a set of pulse widths in Fig. 5.5. In comparison with GaN, the larger thermal conductivity $k$ of the SiC substrate enables longer width of pulsed operation due to the more efficient dissipation of heat generated in the diode channel. The temperature profile is asymmetrical due to the BCs chosen for the cathode and
Figure 5.4: Electric field distributions for a $n^+nn^+$ diode sampled throughout one period $\tau$ ($f = 0.7$ THz) at $t = 0$ (−··), $\tau/5$ (---), $2\tau/5$ (·), $3\tau/5$ (---), and $4\tau/5$ (solid). $L_{ch} = 400$ nm, $L_c = 100$ nm, and the cross sectional area $S = 2500 \mu m^2$.
Figure 5.5: Temperature distribution for the $L_{ch} = 400$ nm GaN diode with a SiC substrate sampled during the "on" portion of the duty cycle.
bottom of the substrate in addition to the highly localized heat generation source. For smaller pulse widths, or during the initial moments of the heating cycle, the diode temperature is almost independent of the substrate thickness and the diode is effectively thermally isolated from the ambient substrate boundary. Consequently, at 0.5 ns the high temperature region is highly localized near the anode junction and the majority of the substrate remains close to the ambient temperature. At later time moments, there is a substantial increase in the temperature maximum and the spreading of the high temperature region towards the cathode and into the substrate. After a pulse width of approximately 3.0 ns the peak temperature approaches the highest allowable temperature of 600 K. The increase in the slope of the temperature distribution in the substrate with time indicates that the diode maintains thermal contact with the heat sink provided at the bottom of the substrate. The dynamic temperature distribution is again shown in Fig. 5.6) for the ”off” state cooling cycle. It is evident that the device must turned off for a few tens of ns to reduce the channel temperature to near its initial state of 300 K. Accordingly, it is necessary to operate the device in the pulsed mode, to avoid critical heating and irreversible degradation, with short pulses of a few ns and a duty cycle of 30-50 ns.

It is favorable to use the lowest possible channel doping density to sustain stationary state oscillations, $N_d = 3 \times 10^{17}$ cm$^{-3}$. Higher densities, necessary for Gunn domain formation, lead to higher current densities and drastically increase dissipated powers and heat generation rates in the diode channel. The considered doping density
Figure 5.6: Temperature distribution for the $L_{ch} = 400$ nm GaN diode with a SiC substrate sampled during the "off" portion of the duty cycle.
corresponds to modes of operation in the absence of Gunn domains and the analysis of the time-dependent carrier distributions confirms operation in the accumulation layer mode.

By adjusting the circuit parameters, it is possible to tune the system to deliver maximum power and efficiency at a specific frequency or to increase the frequency with a lower generated power [112]. In Figs. 5.7 and 5.8, the ac generated power and conversion efficiency as functions of time for a diode with $L_{ch} = 400$ nm and for frequencies corresponding to the peak achievable power at 0.7 THz (a) and maximum possible frequency while maintaining steady state generation at 0.9 THz (b) is shown. The degradation in both power and efficiency correspond to degradation over one pulse width (3 ns for peak power) or for shorter pulses of varying width and a time step of 0.5 ns. Thermal degradation with the SiC substrate is slower than for that of GaN due the larger value of $k$ for SiC. It should be noted that although a reduction of power and efficiency is found for a pulse width of 1 ns, there was little noticeable reduction in operating frequency (less than 5%). Most importantly, while there is a non-negligible reduction of power for longer pulses and the peak temperature in the diode is near the maximum allowable operating temperature, there is still the substantial ac power generation of 2.2 W at 0.7 THz and 40 mW at 0.9 THz.
Figure 5.7: Power $P_{ac}$ and conversion efficiency for the $L_{ch} = 400$ nm GaN diode with GaN and SiC substrates sampled during the "on" portion of the duty cycle for a frequency of $f = 0.7$ THz.
Figure 5.8: Power $P_{ac}$ and conversion efficiency for the $L_{ch} = 400$ nm GaN diode with GaN and SiC substrates sampled during the "on" portion of the duty cycle for a frequency of $f = 0.9$ THz.
5.3 Conclusion

A self-consistent electrothermal model was developed to investigate the effect of thermal degradation on the performance of submicron GaN $n^+nn^+$ diodes operating at THz frequencies. This was accomplished by coupling a time dependent thermal conduction model to an already established electrical drift diffusion model through the temperature dependent electron drift velocity. The effect of Joule heating on the output power and conversion efficiencies was analyzed and the "on"-state and "off"-state pulsed regime widths, necessary to prevent overheating, were estimated. It was found that it was possible to produce an output power of 40 mW at 0.9 THz in the pulsed regime operation, with short pulses of a few ns and a duty cycle of 30-50 ns.

\[1\] This work submitted, in part, in *Appl. Phys. Lett.* [112]
Chapter 6

Conclusion

6.1 Summary of Work

In recent years there has been significant progress in the development of group III-nitride semiconductor devices. These devices have been successfully applied to the generation of high power radio frequency radiation and have led to significant advances into microwave spectrum generation [32]. Further increases in generation frequency are desirable to exploit possible applications in the areas of chemical and solid-state spectroscopy, security screening, and medical imaging, among others. In Chapter 2, a Monte Carlo model was developed with which it is possible to analyze the carrier dynamics and electron distributions in III-nitride bulk semiconductors. In particular, the streaming-carrier regime, characterized by a highly anisotropic electron function due to the dominance of inelastic polar-optical phonon scattering, was examined.
The analysis of the average kinetic energy associated with electron motion transverse to the field, and the mean-square deviation of the longitudinal component of the electron velocity, show that it is possible to achieve a “quasisaturation” region at low temperatures and moderate electric fields. This feature may be exploited in the generation if high frequency electromagnetic radiation [52].

In Chapter 3, the previously developed Monte Carlo model was extended to include the evolution of quantum mechanical electron spin in bulk GaAs. The relevant mechanisms for the spin relaxation in a population of polarized carriers were analyzed and subsequently included in the simulation model. Spin-dependent transport in the drift regime was investigated and the spin relaxation time and characteristic decay lengths at room temperature were determined.

In Chapter 4, a drift diffusion model was developed to determine the conditions for the THz operation of a submicron $n^+nn^+$ GaN diode. The conditions for the generation of THz electromagnetic radiation were analyzed analytically, and a numerical simulation of the diode coupled to an external RLC circuit, was performed to characterize the dynamical electron transport and relevant output parameters. It was found that the diode could operate well into the THz spectrum, with a rather large tuning capability, while maintaining suitable ac generated output powers with reasonable dc-to-RF conversion efficiencies.

In Chapter 5, the aforementioned drift diffusion model was extended to include the effects of temperature degradation on the output performance of a pulse mode
biased submicron $n^+nn^+$ GaN diode with a SiC substrate. The temperature distribution due to Joule heating in the diode channel, as well as the distribution in the SiC substrate, were calculated. This distribution was used to self-consistently model the self-heating effects on the electrical simulation by updating the temperature dependent electron drift velocity. It was found that although there was degradation in the output parameters of the diode, a significant amount of output power could be produced in the THz regime. The appropriate duty cycle was determined to allow stationary operation of the diode within the maximum acceptable channel temperature limits.

6.2 Recommendation for Future Work

There is room for improvement in the operating frequency, output power, and conversion efficiency in the studied $n^+nn^+$ GaN diode. As the diode is scaled to shorter channel lengths, the frequency of operation increases. However, the assumptions made for the use of the quasi-static approximation in the drift-diffusion model become invalid as the diode approaches the ballistic electron limit. It would be a natural, though computationally time consuming, extension of this work simulate the diode using the Monte Carlo method to describe the electron dynamics of ultra-short channel diodes.

The efficiency and output power might also benefit from further engineering of the
diode channel and junction regions. It was noted above that the channel electric field distribution becomes highly inhomogeneous in the region of the drain contact. It may be possible to reduce the maximum value of this field by tailoring the channel doping density. An added benefit of causing the field to become more homogeneous is that it could lead to operation of the diode in the LSA mode. This would be favorable since it is well known that the LSA mode provides increased efficiencies and output powers in GaAs diodes, a phenomenon which should translate to the GaN-based diode as well.

Finally, it is not practical or possible to use planer construction for the resonant feedback circuit necessary for high frequency oscillations. In microwave oscillator design, the common practice is to insert a high frequency NDR diode into a resonant cavity which may be tuned mechanically. And because we are interested in the highly nonhomogenous field and charge distributions common in devices with prominent non-linear transport properties, it is not sufficient to make a constant field approximation as has been done in the past. Therefore, a logical extension of the above work is to incorporate a finite difference time domain model of a resonant structure, coupled to the semiconductor diode. It is not clear that a common mechanical tuned microwave style cavity will be able to provide a sufficiently high quality factor (Q) for oscillation conditions at THz frequencies. It may therefore be necessary to utilize a dielectric resonator with a periodic surface grating structure to provide a suitable Q and allow for the coherent emission of electromagnetic waves in the THz frequency range.


