Thermal Considerations in the Design of D-Band InP Gunn Devices ¹

Ridha Kamoua

Department of Electrical Engineering State University of New York at Stony Brook Stony Brook, NY 11794-2350

Abstract

Recent theoretical and experimental results have established that fundamental mode operation of InP Gunn devices could be obtained over much of the D-Band frequency region [1]. In particular, a design structure with a graded doping profile increasing from the cathode towards the anode has exhibited superior performance over flat doped structures. However, it is observed that experimentally obtained power levels fell short of the theoretical predicted values. Upon mounting the same devices with the graded doping profile on a diamond heat sink instead of a copper heat sink, a considerable increase in the output power was obtained. Typical power levels exceeded 100 mW at 130 GHz [2]. This clearly indicates that thermal effects play a major role in limiting Gunn performance at high frequencies. To accurately take into account heat generation and dissipation in the design of D-Band Gunn devices, a nonisothermal Monte Carlo computer model has been developed. This model accounts for the heat generation and the effect of lattice heating on the electron transport. Simulation results of the graded structure with copper and diamond heat sinks will be presented and compared to the experimental data. In addition, ongoing efforts to further improve the performance through the use of heterojunction cathode injectors will be discussed. It is predicted that more than 140 mW of cw output power could be achieved at 140 GHz with conversion efficiencies exceeding 4%.

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1 Introduction

Solid state millimeter wave sources are generally characterized by low dc to rf conversion efficiencies. As a result most of the dc input power is dissipated as thermal energy which raises the operating temperature of these devices. Higher temperatures degrade the electronic and physical properties of the device. In terms of the electronic properties, the higher temperature increases the rate of phonon scattering which results in lower carrier mobility. At the device level, this translates into a degradation in the efficiency and a decrease in the oscillation frequency. In addition to the effect on carrier transport properties, at high enough lattice temperatures deterioration of the contacts and the semiconductor material occur which eventually result in the failure of the device. For reliable operation the operating temperature should be kept as low as possible. It has been established that the mean failure time decreases exponentially as the temperature increases [1].

One such source, the Gunn oscillator, has demonstrated the capabilities of generating power over much of the D-Band frequency region while still operating in the fundamental mode. A self consistent Monte Carlo model has been developed in order to investigate the performance of Gunn structures with various doping profiles. Simulation results based on this model have shown that structures with graded doping profiles exhibit superior performance to structures with uniform doping in the active region. In particular, a structure with a doping increasing from 7.5×10^{15} cm⁻³ to 2.0×10^{16} cm⁻³ has been fabricated and tested. It is found that good agreement is achieved in the frequency range of oscillation. However, the experimental output power levels were below what the model predicted. This is due to the fact that the model does not account for the heat generation and dissipation in the device in a self consistent manner with the carrier transport.

In this paper, we discuss the development and application of a self consistent model for the simulation of Gunn devices which takes into account thermal effects on carrier transport. Such model, referred to as a non-isothermal model, is based on the ensemble Monte Carlo technique coupled with a heat flow equation. In the remaining sections, we present the formulation and implementation of the model and discuss its application to the simulation of Gunn structures and compare it with experiment.

2 Basic Formulation

The general procedure for non-isothermal simulation of semiconductor devices consists of solving the carrier transport in conjunction with the heat flow equation. In the present model, the carrier transport in the device is described by the ensemble Monte Carlo technique with the following scattering processes: ionized impurity scattering, acoustic phonon scattering, polar optical phonon scattering, intravalley phonon scattering (L-L, X-X), nonequivalent intervalley phonon scattering (Γ -L, Γ -X, X-L), and alloy scattering. These scattering mechanisms are characterized by scattering rates which depend on carrier energy and lattice temperature. Therefore, to reduce the amount of computation time, scattering rates are computed at the beginning of the simulation for various electron energies and lattice temperatures and stored in a lookup table. The scattering rates depend also on temperature through the variation in material parameters (such as band structure). However this effect is not included due to the lack of reliable data on the temperature dependence of these parameters.

For a non-isothermal analysis, we need to consider the energy exchange between electrons and the surrounding environment. This is illustrated in Fig. 1 which pictures the device as a system of electrons and phonons interacting with the contact reservoirs and the external electric field. In this picture, we have neglected interaction with photons and recombination generation mechanisms. The electron system consists of all conduction electrons in the semiconductor device. With no external forces, electrons are in thermal equilibrium with the lattice. As a result of applying an external force, electrons gain energy from the electric field and lose energy to the lattice due to phonon scattering. In order to account for thermal



Figure 1: Energy picture of the Gunn device.

heating of the lattice, we need to consider the phonon transport problem. This could be described by a Boltzmann Transport Equation (BTE). In a similar approach commonly adopted to describe electron transport, we can derive a balance equation for the internal lattice energy by multiplying the BTE by phonon energy and averaging over the Brillouin zone. The resulting equation, referred to as the heat flow equation, expresses continuity of the internal lattice energy and takes the form of:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla (-\kappa \nabla T) = Q, \qquad (1)$$

where ρ is the mass density, κ is the thermal conductivity, C_p is the specific heat, and Q is the internal power dissipation per unit volume. Q represents the energy exchange between the lattice and the carriers in the semiconductor. The power dissipation density is often modeled by a Joule heating term (product of current density and electric field) which represents the rate of energy gained by carriers from the electric field. In fact, it is more accurately described by the energy exchange between carriers and the lattice[2].

In the present model, the net energy exchange between the lattice and electrons is identified as the heat generation within the lattice. In the Monte Carlo simulation, the net phonon generation per unit volume at cell i and time t is computed according to the

following expression:

$$Q_i(t) = \frac{1}{\Delta t} \left[\sum_{j=1}^{NSE_i} \hbar w_e - \sum_{j=1}^{NSA_i} \hbar w_a \right] A,$$
(2)

where Δt is a time interval around t, NSE_i is the number of scatterings involving phonon emission in cell *i* over the time interval Δt , NSA_i is the number of scatterings involving phonon absorption in cell *i* over the time interval Δt , $\hbar\omega_e$ is the energy of the emitted phonon, $\hbar\omega_a$ is the energy of the absorbed phonon, and *A* is a multiplication factor. The power dissipation density changes at a rate comparable to the oscillation frequency whereas the lattice response time is of the order of few hundred nanoseconds [3]. As a result, the lattice temperature is unable to respond to the rapid changes in the power dissipation density Q(t). With this assumption, it can be shown [4] that we can replace Q(t) with its average over an oscillation period $\langle Q(t) \rangle$. In addition since we are interested in the stationary lattice temperature profile, it is appropriate to consider the steady state heat flow equation. which is expressed in discrete form as:

$$\alpha T_{i-1} - (\beta + \alpha)T_i + \beta T_{i+1} = -\langle Q_i(t) \rangle, \tag{3}$$

where $\alpha = (\kappa_{i-\frac{1}{2}})/(\Delta z)^2$, $\beta = (\kappa_{i+\frac{1}{2}})/(\Delta z)^2$, and Δz is the cell size.

During the simulation process of Gunn devices, the structure, biasing condition, and operating frequency are specified as input parameters while the rf power, efficiency and lattice temperature are output quantities. The program proceeds with the simulation for a number of oscillation periods until a satisfactory solution is achieved. The algorithm of the implemented nonisothermal Monte Carlo program consists of the following steps:

- 1. Start with an initial lattice temperature profile and assign the state of each electron in the ensemble.
- 2. Carry out the ensemble Monte Carlo simulation for one period. Compute the power dissipation density Q_i at each cell in the device and at each time step according to equation 2.

- 3. Determine the average power dissipation density $\langle Q_i \rangle$ over the last period at each cell in the device.
- 4. Solve the heat flow equation for the new lattice temperature profile T_i across the device according to equation 3.
- 5. Repeat from step 2 with scattering rates and material parameters corresponding to the new lattice temperature until a stable solution is obtained.

3 Application to Gunn Device Simulation

In this section, we illustrate the application of the non-isothermal model to the analysis and design of Gunn devices. A typical Gunn device mounted on a heat sink is shown in Fig. 2. In order to solve the heat flow equation, a boundary condition needs to be specified at each



Figure 2: Gunn device on a heat sink.

of the two ohmic contacts. For the top contact, it is assumed that the heat through the

bonding wire is negligible compared to the heat flow towards the heat sink. This assumption implies that the temperature across the top ohmic contact is uniform, i.e., $(\partial T/\partial z) = 0$. For the other boundary between the integral heat sink and the ohmic contact, the temperature at the center of the interface is expressed as [5]:

$$T(IHS) = \mathcal{P}\left(\frac{t_{IHS}}{\kappa_{IHS}} + \frac{R}{\kappa_{HSK}}\right) + T_{amb},\tag{4}$$

where R is radius of the diode, T_{amb} is the ambient temperature, κ_{HSK} is the heat sink thermal conductivity, κ_{IHS} is the integral heat sink thermal conductivity, and \mathcal{P} is the dissipated power per unit volume in the semiconductor region.

4 Simulation of Graded-Doping Gunn Structure

The first Gunn structure considered is similar to the structure realized experimentally. It consists of a 1 μ m InP active region with a doping profile increasing from the cathode to the anode. In order to take advantage of the nonuniform doping profile, the cathode has to be placed near the low doped side. Two configurations for mounting the devices on a heat sink were considered. The first configuration, referred to as heat sink negative, corresponds to the heat sink close to the low end of the graded doping profile. The second configuration, referred to as heat sink positive, corresponds to the heat sink near the high end of the graded doping profile. Simulations were performed using the non-isothermal Monte Carlo model with devices mounted on copper and diamond heat sinks.

4.1 Devices on Copper Heat Sink

The graded structure was simulated with a negative heat sink configuration (heat sink near cathode). The following results correspond to a diode with 45 μ m diameter, biased at a dc voltage of 4.1 V and operating at 132 GHz. Figure 3 (a) shows the lattice temperature across the device as it evolves over many periods. A converging solution emerges after only



Figure 3: (a) evolution of lattice temperature over many periods in a graded-doping structure with a copper heat sink, (b) lattice temperature profile in devices with diameters of 40 and 45 μ m.

few periods and corresponds to a cathode temperature of 420 0 K and anode temperature of 452 0 K. The simulation predicts an output rf power of 53 mW with a conversion efficiency of 2.2 % and a dc current of 590 mA. Experimentally, it was observed that for a reasonable rate of success in packaging InP Gunn diodes on copper heat sink, devices with diameters of 40 μ m or less are required. Figure 3 (b) shows that the maximum temperature in a 40 μ m diode is ten degrees lower than the corresponding temperature in a 45 μ m diode. For the same biasing condition and oscillation frequency, the smaller structure yields a power of 42 mW with 2.2 % efficiency and a dc current of 470 mA. Based on these results, it appears that for reliable operation of InP Gunn devices, the lattice temperature should be kept below 450 0 K. With this thermal limitation, more power could be extracted by either using a better heat sink or improving the efficiency of the device. These two options will be considered in the following sections.

4.2 Devices on Diamond Heat Sink

In this section, the graded structure is simulated with a diamond heat sink. Diamond has a much higher thermal conductivity compared to copper. Therefore it is possible to use larger devices and still maintain the operating temperature below 450 °K. Figure 4 illustrates the lattice temperature profile for a 55 μ m diameter device under the same biasing condition and frequency of operation as in the previous section. Figure 4 (a) corresponds to a diode with the heat sink at the anode side, whereas in fig. 4 (b) the heat sink is at the cathode side. In the case of heat sink at the anode (heat sink positive), the lattice temperature increases from 395 °K near the anode to 410 °K near the cathode. On the other hand, when the heat sink is at the cathode (negative heat sink), the temperature peaks near the anode and reaches a value of 428 °K. This implies that the heat sink in a graded structure should be



Figure 4: Lattice temperature across a 55 μ m diameter diode on a diamond heat sink. (a) heat sink at the anode, (b) heat sink at the cathode.

placed at the anode contact. Such a configuration results in a lower operating temperature because the heat sink is adjacent to the region in the device where most of the heat is generated. This is clearly illustrated in fig. 5 where the power dissipation density across the diode is shown (anode is located at 1.4 μ m). With this configuration, the simulation predicts an output power of 103 mW at 132 GHz, a conversion efficiency of 2.7%, and a dc current of 0.93 A. These results are in good agreement with experimental data [6] where the measured efficiency at 132 GHz was 2.5 %. The same Gunn structure was simulated with a negative diamond heat. The model predicts slightly less power than obtained in the positive heat sink configuration by about 5 to 10 mW.



Figure 5: Power dissipation density across a 55 μ m diameter diode with a positive diamond heat sink.

5 Simulation of Heterojunction-Cathode Structures

In this section, we investigate an InP Gunn structure with a heterojunction injector consisting of an InGaAs barrier region. For proper operation, the heterojunction injector should be the cathode. In this configuration, a large electric field occurs near the cathode which contributes to the reduction of the dead zone and therefore improves the efficiency of the device [7]. Simulations were carried out on a structure designed for operation at 140 GHz which is the frequency of interest in an ongoing project. The structure consists of a 0.8 μ m active region doped at 2 × 10¹⁶ cm⁻³ with a 125 meV barrier. Figure 6 shows the lattice temperature profile along a 55 μ m diameter device with a positive diamond heat sink and a dc bias of 3.9 V. The maximum temperature occurs at the cathode and is only 400 °K. The simulation predicts an output power level of 140 mW with 4.2 % efficiency and a dc current of 0.85A. The low temperature is a result of the smaller current density and the higher



Figure 6: Lattice temperature along a heterojunction cathode InP Gunn structure with positive diamond heat sink. The device has a diameter of 55 μ m and is biased at a dc voltage of 3.9V.

efficiency compared to the graded structure. The improvement in efficiency is attributed to the effectiveness of the heterojunction barrier in providing electrons enough energy to transfer to the upper energy valleys. Figure 7 compares the maximum fraction of electrons in the upper valleys along the active region for the the graded and heterojunction cathode structures. Although the length of the active region is not the same, it is clear that in the heterojunction cathode structure the fraction of electrons in the upper valley is much higher near the cathode.



Figure 7: Fraction of electrons in upper energy valleys: (a) heterojunction cathode structure, (b) graded structure.

6 Conclusion

A non-isothermal Monte Carlo model for the simulation of InP Gunn devices has been developed. It is based on the ensemble Monte Carlo technique coupled with a heat flow equation. A Gunn structure with graded doping profile was simulated using this model. It was found that diodes should be limited to 40 μ m in diameter when a copper heat sink is used in order to keep the temperature below 450 °K. With a diamond heat sink, the model predicts an operating temperature below 450 °K for a 55 μ m diode with a performance in good agreement with experimental measurements. Finally, a structure with a heterojunction cathode injector results in 50% improvement in efficiency and output power while operating at a lower temperature compared to the graded structure.

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