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Monte Carlo modelling of multiple-transit-region Gunn diodes

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Abstract
Our Monte Carlo model shows that the incorporation of multiple transit regions into a single Gunn device is a feasible means of increasing the output power of the device. From our simulations, the power attainable from these multiple-transit-region Gunn diodes increases linearly with the square of the number of transit regions, while the efficiency remains approximately the same. We have found that the coherent transfer of domains occurs in all the investigated devices (up to eight transit regions). There seems to be no obvious upper limit to the number of transit regions that can be incorporated into a single device (in the absence of thermal limitations).

1. Introduction

The Gunn diode, sometimes referred to as a negative differential resistance (NDR) device, has been a popular microwave frequency source since the 1970s [1–3]. Currently, it is the preferred route to the provision of 50 mW of power at 77 GHz in automotive adaptive cruise control (ACC) radars, which are being fitted to a number of cars. Although in direct competition with monolithic microwave integrated circuit (MMIC) technology and hybrid Gunn diode/MMIC systems, these devices offer the advantages of higher power, higher definition, greater range and far better system linearity in the frequency sweep with lower phase noise and higher accuracy, together with a greater mechanical robustness. The Gunn diode is very small, with a chip diameter of 0.3 mm. It is now available in the form of a surface-mounted voltage controlled oscillator (VCO) with low phase noise and it has excellent performance over a wide range of temperatures.

To date, conventional Gunn diodes consist of a single transit region, the length of which is determined by the time T taken for a charge monopole or dipole to transfer from the cathode to the anode at approximately 10^5 m s^{-1}. The fundamental frequency is approximately given by 10^5 m s^{-1}/L Hz, where L is the length of device. Gunn diodes used for high-frequency generation ($\sim$100 GHz) therefore need to be quite short ($\sim$1 μm) if they are to operate in their fundamental mode. This limits the amount of power that the devices are capable of producing because of the small potential that can be applied. For this reason, these devices are frequently used in the second-harmonic mode where they are designed with a transit time of twice the inverse operating frequency [4]. Most designs use the second-harmonic oscillation to achieve $\sim$100 GHz and powers of up to 80 mW at 90 GHz, and 2.4% efficiency has been demonstrated at room temperature [5].

Fundamental mode operation, however, gives higher efficiency and power and is therefore preferable. As such, much effort [6, 7] has been made to increase the output power of these diodes, for example, mounting devices in parallel in the cavity, known as 'power combining' [8]. Unfortunately, the diodes must be positioned very precisely at an integer number of wavelengths apart. This increases the complexity of the architecture of the system and the number of components required, thus making this an expensive option.

There is, however, a simple way around this 'low potential' problem. If we could place two or more diodes in series, and if they could operate coherently, then in principle a higher potential could be applied. A single device with multiple transit regions would therefore be an efficient way of solving this problem. Physically linking discrete devices may be possible, though inductance effects in the linkage may affect the phase relationship between them. Such multiple-transit-region Gunn diodes were first proposed by Tsay *et al* [9], but very little work has subsequently been done on this idea. Indeed, we are aware of only one other publication which has reported on simulations of double-transit-region Gunn diodes [10].

In this paper, we investigate the power performance of Gunn diodes of up to eight transit regions and we also investigate the effect of manufacturing variability on the performance of these devices. The paper is organized as

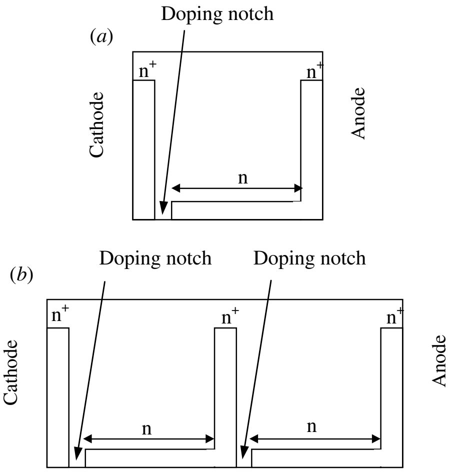

Figure 1. Schematic diagrams of the doping profiles of the simulated devices for (*a*) single transit region and (*b*) double transit region.

follows. In section 2, we describe the methods employed and the devices simulated. In section 3, we present results obtained from our simulations, followed by our conclusions in section 4.

2. Method

Of the simulation techniques currently used for semiconductor device modelling, the Monte Carlo method provides a means of gaining a strong physical insight into both the behaviour of semiconductor materials and the operation of small-scale devices. Compared to drift–diffusion simulation models, the Monte Carlo model is capable of providing a more accurate solution of the Boltzmann transport equation. The accuracy in the physical description, however, comes at the cost of a high degree of computing power and the results are a little noisy, due to the stochastic nature of this method.

The method simulates the motions of charge carriers through a semiconductor device. These particles are propagated classically between collisions according to their velocity, effective mass and the prevailing field. The selection of the propagation time, scatter mechanism and the states after scattering are achieved by the generation of random numbers. A thorough description of the method can be found in [11].

We have simulated multiple-transit-region Gunn diodes by using a one-dimensional self-consistent ensemble Monte Carlo model. A detailed description of the method has been given in [12] where an extremely good description of high field transport in GaAs can be found. Each simulation was performed with 30 000 super particles on a mesh of 3 nm with a field adjusting time step of 0.1 fs.

2.1. *Simulated devices*

We have simulated conventional single-transit-region GaAs Gunn diodes with the doping profile as shown in figure 1(*a*). For all the simulations carried out, the active region is sandwiched between the highly-doped n^+ (1×10^{24} m^{-3}) cathode and anode regions. A device diameter of 75 μm has been assumed in all our simulations. A doping notch is incorporated at the beginning of the transit region of the Gunn diode to stimulate dipole formation near the cathode. The dipole is encouraged to form at this point as the doping discontinuity causes an increase in electric field [13]. It is vital to have a doping notch that is just wide enough for dipole nucleation. Our simulations indicate that, with a doping notch of 0.1 μm, our Gunn diode starts to work in an accumulation mode. When the notch is 0.4 μm, a very defined dipole domain is formed initially but further formation of domains is hampered as this 0.4 μm notch acts as a resistive element in the device. From our investigation, we have found that the devices oscillate in a dipole mode when we use a doping notch of 0.2 μm; this is the length of notch that we use for all subsequent simulations.

The condition of $nL > 10^{12}$ cm^{-2}, where n is the doping density and L is the length of the transit region, must be satisfied for a Gunn domain to form. Typical Gunn devices for millimetre wave generation have nL products between 1×10^{12} cm^{-2} and 3×10^{12} cm^{-2} [2]. The higher the doping density of the transit region, the easier it is for the domains to nucleate and grow. However, a high density will cause the device to overheat and burn out quickly. As a compromise, we have used a doping density of 1.5×10^{22} m^{-3} at which the devices were found to operate reasonably well.

To determine the relationship of the transit region length and the natural frequency of operation, we simulated devices of different lengths of the n region (1–2 μm) with a 5 V dc potential being applied at the contacts. For subsequent simulations, we have chosen 1.3 μm as the transit region length, giving an nL product of 1.95×10^{12} cm^{-2} which is about the midpoint of operation for typical Gunn diodes in the frequency range we are interested in. Because we are investigating a novel form of Gunn device, we are only interested, at this stage, in investigating and establishing the fundamental operating principles. For this reason, we have chosen a relatively 'long' device (50 GHz), rather than one that is of more commercial interest (77 GHz or 94 GHz) but is shorter and more demanding to grow and fabricate.

As heat generation and temperature gradients are significant as devices get longer, the effect of temperature on the frequency response of the Gunn diodes is of particular interest [14]. We have therefore simulated the operation of the Gunn diodes working at temperatures between 300–450 K.

For the double-transit-region devices, the doping profile used in the simulation is shown in figure 1(*b*). Here, another identical transit region is added to that in figure 1(*a*). We have used the same doping density as before. For all subsequent simulations of more than two transit regions, we have added additional transit regions with the specifications of the double transit region as shown in figure 1(*b*).

So far, we have simulated ideal devices that have exactly identical features. A question of particular interest is whether these devices would still work under more realistic fabrication conditions; for example, a double-transit-region device which has transit regions that are of slightly different lengths, differing by as much as 10%. For this reason, we have simulated a two-transit-region Gunn diode with transit region lengths of 1.3 μm and 1.4 μm in the first and second regions, respectively.

2.2. Power calculation

A sinusoidal driving potential imposed on a dc bias has been assumed in order to mimic the effect of placing the device in a radio-frequency (rf) cavity [15]. A dc bias of 5 V and a rf bias of ± 2 V are applied for a single transit region.

The sinusoidal input voltage is given as

$$V(t) = V_{\mathrm{DC}} + V_{\mathrm{RF}} \sin(2\pi f t), \tag{1}$$

where V_{DC} is the imposed dc potential, V_{RF} is the ac potential, and f is the frequency of the sinusoidal waveform. From the output current obtained from the Monte Carlo simulations, the output power is calculated as follows. The rf power output P is given as

$$P_{\mathrm{RF}} = \frac{V_{\mathrm{RF}}}{2} \times \frac{2}{T_{\mathrm{R}}} \int_0^{T_{\mathrm{R}}} i(t) \cos\left(\frac{2\pi t}{T_{\mathrm{R}}}\right) \mathrm{d}t \tag{2}$$

and

$$T_{\mathrm{R}} = \frac{1}{f}. \tag{3}$$

The integral provides the current amplitude in antiphase with the rf voltage $V(t)$. Similarly, the dc power dissipation in the device is

$$P_{\mathrm{DC}} = V_{\mathrm{DC}} \times \frac{1}{T_{\mathrm{R}}} \int_0^{T_{\mathrm{R}}} i(t)\, \mathrm{d}t \tag{4}$$

and the rf efficiency is given by

$$\eta = \frac{P_{\mathrm{RF}}}{P_{\mathrm{DC}}}. \tag{5}$$

For the power calculations, the devices were simulated for a period of about 100 ps (equivalent to about four domain transits/cycles) and the current obtained by averaging over every 10 fs.

The resistive impedance, Z_{R}, and the reactive impedance, Z_{X}, are given as

$$Z_{\mathrm{R}} = V_{\mathrm{RF}} \frac{a}{a^2 + b^2} \tag{6}$$

$$Z_{\mathrm{X}} = V_{\mathrm{RF}} \frac{b}{a^2 + b^2} \tag{7}$$

where

$$a = \frac{2}{T_{\mathrm{R}}} \int_0^{T_{\mathrm{R}}} i(t) \cos\left(\frac{2\pi t}{T_{\mathrm{R}}}\right) \mathrm{d}t \tag{8}$$

and

$$b = \frac{2}{T_{\mathrm{R}}} \int_0^{T_{\mathrm{R}}} i(t) \sin\left(\frac{2\pi t}{T_R}\right) \mathrm{d}t. \tag{9}$$

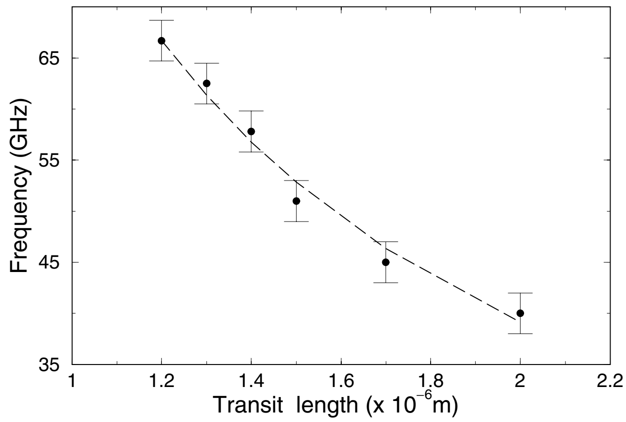

Figure 2. The natural frequency of oscillations as a function of active n region length at a temperature of 450 K.

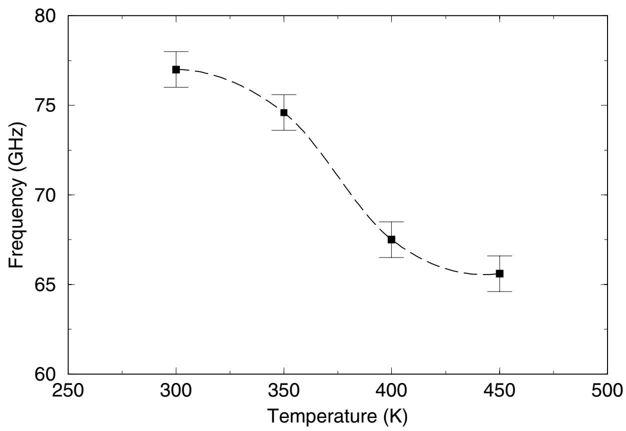

Figure 3. The natural frequency of oscillations as a function of temperature.

3. Results and discussion

3.1. Single transit region

In this simple device, Gunn domains form at the notch and propagate through the transit region. Figure 2 shows that the longer the transit region, the longer it takes the domain to travel, and hence the lower the frequency. The graph shows that the natural frequency response is approximately the inverse of the transit region length of the device. By varying the operating temperature of our device, we have found that, as the temperature increases, scattering becomes more prominent and causes the domains to move across the device more slowly, resulting in a decrease in the natural frequency of the output current as shown in figure 3.

3.2. Two transit region

Essentially, the domain forms and travels across the device in a similar way as in a conventional Gunn diode. In a single-transit-region device, when a Gunn domain exits through the anode, charge is lost from the region and the potential associated with the domain redistributes across the entire transit region. This increases the field into the negative differential resistive regime of the material, thus allowing a new domain to nucleate at the cathode. In multiple-transit-region devices, we can see that the potential redistributes across all the regions evenly with each domain in each transit region behaving as if it is in a single-transit-region device. Figure 5 shows successive distributions of the electric field and electron density, where we have obtained almost identical Gunn domains forming and transferring coherently in each of the regions.

From the simulation it can be seen that, by using this design, a higher potential can be applied and hence higher power achieved. Figure 4 shows that, for a double transit region, the power obtained is twice that of a single-transit-region device for favourable frequency ranges. The efficiency is just marginally higher than that we obtained from a single transit region, though the reason for this is unclear.

Figure 6 compares the frequency responses of the Gunn diodes operating at different temperatures. As expected from our earlier results shown in figure 3, the optimum operating frequency decreases as the device becomes hotter and the maximum output power obtainable decreases as temperature increases.

Our investigation so far has assumed that perfect devices are fabricated. To consider a more practical scenario, we have incorporated some errors into the simulated devices to investigate their operation. Our results have revealed that, even after anticipating fabrication inaccuracies in making the device, a double-transit-region device with different transit region lengths still works reasonably well. With a device that has transit region lengths of 1.3 μm and 1.4 μm, current oscillations with a slight decrease in the frequency are obtained. This is due to the fact that the device is now slightly longer compared to the device with equal transit region lengths of 1.3 μm.

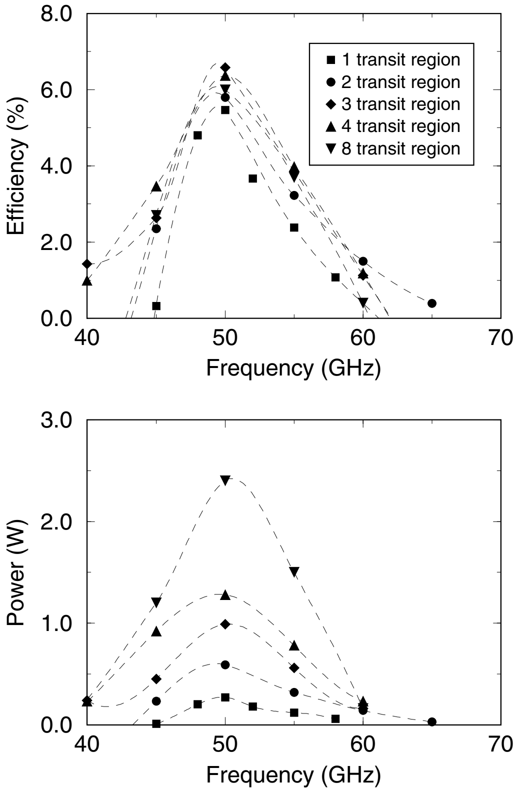

Figure 4. The power and efficiency as a function of frequency of the input sinusoidal potential for one, two, three, four and eight transit regions. The lines are drawn to guide the eye.

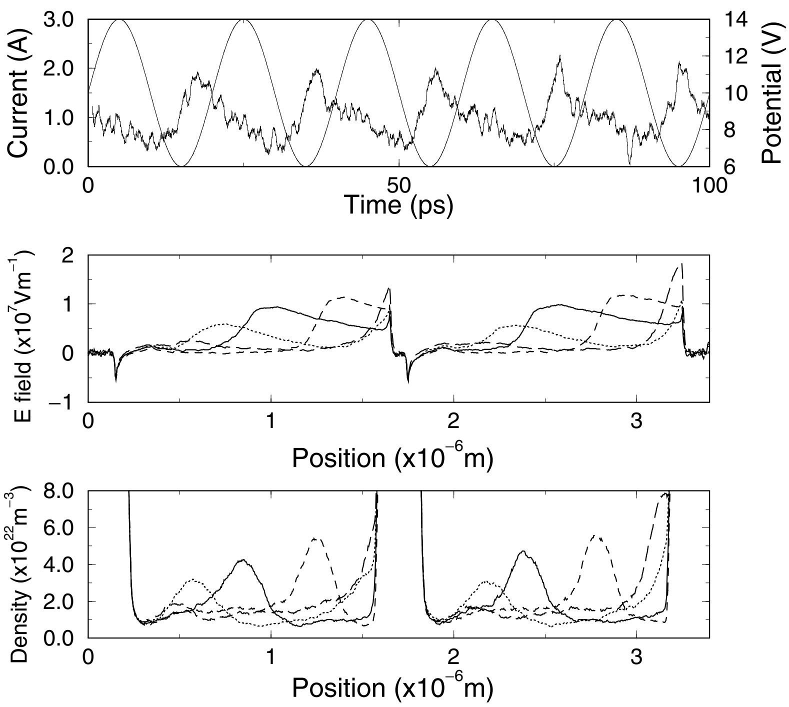

Figure 5. The electric current and applied potential (smooth line) (50 GHz, 10 V $\pm$ 4 V) (top), electric field and charge density at the times, 43 ps (——), 56 ps (- - - -), 69 ps (- - - -) and 73 ps ($\cdots\cdots$), in a double-transit-region device.

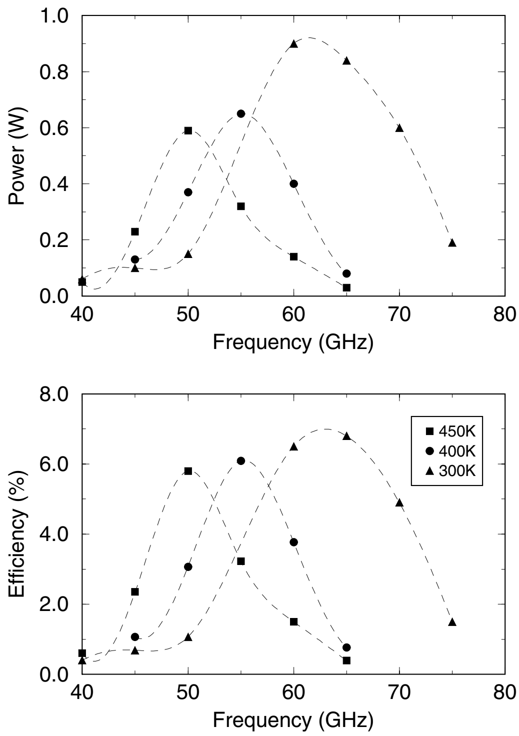

Figure 6. The power and efficiency as a function of frequency of the input sinusoidal potential for temperatures of 300, 400 and 450 K. The lines are drawn to guide the eye.

3.3. Three to eight transit regions

We continued on to simulate devices with three, four and eight transit regions and to investigate their performances. Figure 7 shows successive distributions of the electric field and electron density for a three-transit-region device where we obtained almost identical Gunn domains forming and transferring coherently in each of the regions.

As in the case of the two-transit-region Gunn diodes, the domains are found to form and travel coherently in all the simulated devices. The potential applied across an N-transit-region device can be N times that of a single-transit-region device. Figure 4 compares the power and efficiency obtained from our simulated multiple-transit-region diodes. From these results, we can predict that the output power of the multiple-transit-region device is found to be proportional to the number of transit regions of the device (with the external voltage applied) while the efficiencies remain approximately the same. However, the theoretical maximum power assuming temperature uniformity, for N transit regions is actually N^2 times as much power at a given frequency as a conventional single-transit-region Gunn diode [9].

In our simulations, for the sake of simplicity and ease of comparison, the cross section of each device has not been increased. The reason for this improvement is that an N-transit-region diode has N times the impedance of a single-transit-region diode. Figure 8 compares the resistive and reactive impedance of all the simulated multiple-transit-region devices. The cross-section area can be increased by a factor of N, not exceeding the maximum value of conductance, without excessive circuit loss.

From our results, we have not found any obvious upper limit on the number of transit regions. Although theoretically it is possible to build a device with any number of transit regions, the implementations of such long Gunn diodes may generate a high amount of heat and induce temperature gradients within

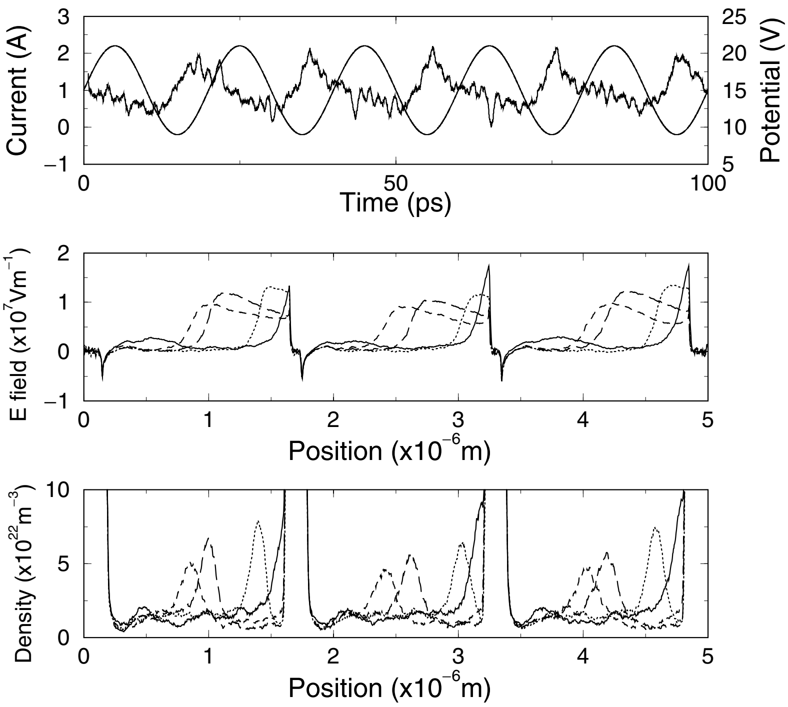

Figure 7. The electric current and applied potential (smooth line) (50 GHz, 15 V $\pm$ 6 V) (top), electric field and charge density at the times, 53 ps (——), 56 ps (- - - -), 67 ps (- - - -) and 73 ps (· · · · · ·), in a triple-transit-region device.

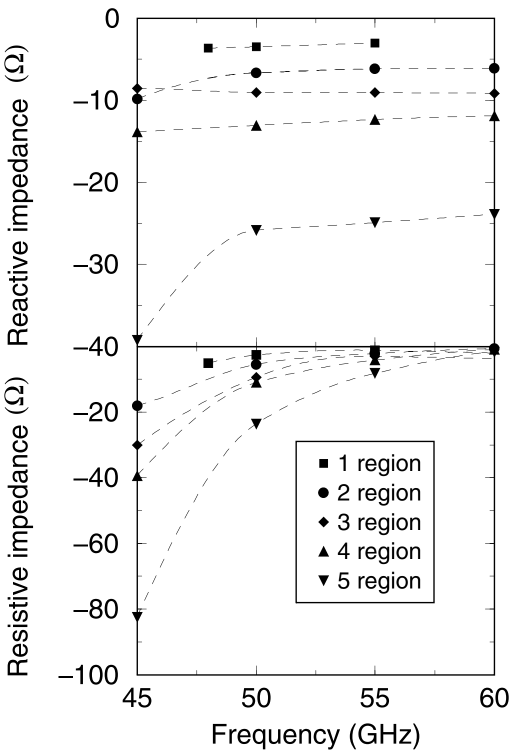

Figure 8. The resistive and reactive impedance as a function of frequency of the input sinusoidal potential for one, two, three, four and eight transit regions.

the semiconductor that may affect the operation of these devices.

4. Conclusion

Our results illustrate the incorporation of multiple domain transit regions in a single diode as a feasible means of overcoming the 'low power' problem associated with the device operating at high frequencies. Using this method, the potential across the device can be substantially increased with a corresponding increase in power attainable. The device will be able to function in a fundamental mode (in each of the transit regions). Despite the increase in the length of the device, higher efficiencies associated with the fundamental mode operation can be achieved. Our results predict that the power attainable by an N-transit-region Gunn diode could be up to N^2 times that of the corresponding single-transit-region device when oscillating in its optimum frequency in the absence of heat limitations. We have also shown that these diodes still perform well after taking into account the fabrication of non-identical transit regions.

The development of these devices is currently in progress and we will report shortly on the first such devices to be fabricated. The use of smaller multiple transit regions will enable the device to be used in the fundamental mode and to deliver more power. A further consequence is that a useful level of power will be available at the second harmonic which will be ∼150 GHz. The realisation of such multiple-transit-region diodes would be a significant and exciting advancement in Gunn diode technology, which would widen the realm of device applications for these diodes; especially for higher-frequency applications, such as ACC radars, which are of great current interest in western Europe and the USA where the anticipated market value is anticipated to reach about $6 billion pa by 2005 [16].

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