Abstract—A novel gallium arsenide (GaAs) planar Gunn diode design with shaped anode and cathode contacts using Monte Carlo simulations has been shown to produce significantly higher frequency fine structure components in the output waveform than the natural transit time frequency of the diode. We have investigated devices operating both with and without feedback potential (in delayed mode) and have shown 350 GHz fine structure frequency components in a device with a nominal transit time frequency of 70GHz is possible. This is the first observation of such stable repeating high frequency components in a Gunn diode, giving potential for very high frequency power generation and other wave shaping applications.

Index Terms—GaAs, Planar Gunn diode, Monte Carlo, Multiple peaks, High frequency
simulations showed that sharp corners can lead to poorly formed and distorted domains. It was found that this could be corrected by shaping the contact corners to reduce the strength of the field [11].

Planar Gunn diodes offer the possibility of exploring other novel contact shaping which differs from the morphology of the default linear parallel design of the cathode and anode. Very small feature sizes are possible allowing intricate designs to be investigated and the technology to achieve this will be discussed in section III-D. Circular geometries were explored in [12], while investigations into different sizes of anode and cathode in a vertical Gunn geometry have been published in [13]. Simulations of a crenellated cathode in [14] showed the curious effect on the shape of the domain of this non-parallel design.

The natural fundamental frequency of a planar Gunn diode is determined by the width of the channel and the velocity of the domain. As the channel region width becomes shorter, there is less room for the domain to form and meeting the well known nl (channel doping x channel width) product rule [15] which limits the frequency of operation of a Gunn diode. Fabricating devices smaller than one micron is difficult, as the electron densities for good operation need to be high and such devices suffer from undesirable heating effects in the channel region.

To overcome this limitation, one idea that presents itself, is for a single Gunn domain to be incident on a shaped anode giving a graded channel width thereby the domain hits this contact multiple times, each time causing an increase in current. The current output of such a device would no longer be solely dependent on the period of time of transit, but would have frequency components dependent on the separation of the points of contact between the cathode and shaped anode which might possibly be considerably shorter than the width of the channel.

However, in a normal Planar Gunn with a perfectly straight anode, the shape of the sharp corner at the edge of the channel can have an important effect on the shape of the Gunn domain as discussed earlier. Introducing more complicated shaping of the anode may cause chaotic dynamics within the device with the domain forming and reforming in ever more complicated shapes on each subsequent transit. In [16] a shaped cathode was shown to produce a very complicated current waveform, probably from the aforementioned chaotic dynamics, and when analyzed was found to contain many frequency components.

In this paper, using an ensemble Monte Carlo method, we will demonstrate a planar Gunn diode design that produces stable, repeating domains yielding a simple current waveform with multiple peaks corresponding to each transit of the domain. This was achieved using a simple applied DC potential without feedback and a delayed mode transit with feedback [17,18].

II. DEVICE DESIGN AND SIMULATION

An ensemble Monte Carlo method was used to simulate the carrier transport in the studied devices with an established 2-D Ensemble Monte Carlo (EMC) transport model, details of which are given in [19], which has been validated against many similar experimentally realized devices [2,3]. As in [14] a doping notch next to the cathode contact was used to simulate the effect of the cathode contact to precipitate domain formation. A typical mesh of 100 by 100 was used with up to 500,000 super particles. Each super-particle represents a number of real particles such that the charge carried by the super-particles will reproduce the correct charge density which is then used to calculate the electric field in each field adjusting timestep. These particles are propagated classically between collisions according to their velocity, effective mass and the prevailing electric field in the standard manner [20]. All electrons were weighted equally, and a typical run time was about 12 hours to simulate 50ps. A field adjusting time step of 1 fs was used and the boundary conditions adopted were the usual Dirichlet conditions at the contacts with defined potentials and Neumann conditions at other boundaries assuming continuity of the electric field. For the DC calculations an impressed voltage VDC was applied at the contacts as the boundary conditions. A recognised drawback of Monte Carlo modelling is the statistical (noisy) nature of the simulated current. It is this feature that makes linking a Monte Carlo model with an external circuit model difficult [21]. For devices in a resonant circuit therefore, the interaction of the device and the circuit is described by assuming that steady-state oscillations have been established and the diode is driven by a known RF voltage VRF such that $V = V_{DC} + V_{RF} \sin(\omega t)$ in the standard manner [21, 22, 23 and 24]. To improve the statistics in the present study, the current I(t) through the device was evaluated by averaging the charge output through each contact (the number of super-particles passing through the contact together with displacement current) at each field adjusting time step over 40 output values, which equates to less than 0.1 ps. This is much less than the time-period of the oscillations for the frequencies of interest (up to 350 GHz corresponding to a time-period of ~2.8ps).

We simulated a whole planar Gunn diode with a 24 um of channel length. A schematic of the simulated structure is shown in figure 1 and the process of arriving at this design will be discussed in section III-A. Devices with channel widths $L_1$ ranging from 1.30 - 1.60 um and $L_2$ ranging from 1.44 - 1.46 um, were investigated. As in [11], the simulations were done on the presumption of a lattice temperature of 300 K (room temperature).

![Fig. 1. Schematic of the novel planar Gunn diodes used here in the simulations.](image-url)
Results will be presented for both transit time and delayed mode oscillations. In the transit mode, the device is biased with a constant applied potential. For delayed mode oscillations, there is a substantial AC feedback component (1V) on a 2V DC component so that wherein the potential after each transit drops below the threshold for domain formation. A new domain will reform at the anode as the potential increases above the threshold again.

III. ANALYSIS AND DISCUSSION OF RESULTS

A. Preliminary investigation of contact shaping

Before discussing the results of the designed device, it is important to explain how the design was arrived at. Figure 2 shows a schematic illustration of the evolution of the design starting with a simple crenellated geometry (figure 2a). The descriptive terminology is defined as follows, in a crenellation the merlons are the “fingers” that extends toward the other electrode and the gaps between the fingers are the crenels (see figure 2a). In this design it was found that a domain traveling from the cathode will first be incident on the leading edge of the anode, or merlon. As the domain advances into the crenel it wraps around the merlon until finally it hits the bottom recess of the crenel. Because of the domain wrapping around the merlon, the current increase was found to be smooth and continuous, rather than delivering two distinct peaks of current corresponding to hitting the leading edge of the merlon and then the bottom recess of the crenel. In order to reduce the wrapping effect, attempts were made to shape the merlon in the form of a dovetail (figure 2b) which did improve the operation of the device and increased improvements were achieved by further hollowing out the merlon (figure 2c). The smallest feature size on the anode is about 100nm which is experimentally realisable and this will be discussed in section III-D.

Fig. 2. (a) schematic of the crenellated design anode contact. (b) schematic of the dovetail shape anode contact. (c) schematic of the novel contacts planar Gunn diodes analyzed in this work.

Returning to the simple crenellated design, as the domains hit the merlon, partial domains reform at the cathode opposite the merlons. Only when the rest of the domain passes through the bottom of the crenel do the corresponding parts of the domain reform at the cathode, by which time the merlon parts of the domain have already made some progress on their transit. In this way, the newly formed domain is considerably distorted, and this distortion grows with each subsequent transit, eventually leading to chaotic current output. The merlon and crenel parts of the diode have different channel widths and the domain structure and output current consequently become very complicated and out of phase with each other.

The obvious solution to this, is to operate the device in a delayed mode. In this mode the feedback potential is such as to allow the potential to fall below the threshold value for domain formation, thus extinguishing any incipient domain at the anode. When the voltage once again increases above the threshold, a new fresh domain can reform which will not suffer from any memory of previous transits. This mode of operation will be discussed in section III-C.

Another means by which the different period problem can be mitigated is by using the negative differential resistivity of the electron transport. The shorter distance between the anode and cathode of the merlon part of the device leads to a higher field, and a more slowly moving domain. The greater distance between anode and cathode in the crenel portion, has a lower electric field and consequently faster domain, by careful selection of the applied bias and the distances between anode and cathode, a point of stationary transit time can be found where despite small differences in distance, the transit period is the same and so the different parts of the device can maintain a stationary phase difference with each other. Normal Gunn diodes will operate from their threshold to when breakdown occurs, which will give a voltage range of about 4V, (depending on their size). However, the requirement for stationary transit time reduces this range to about 0.5V. Here we found that the range of operating voltages was between 1.8 - 2.3V with an optimal voltage of 2V. We also found that including a merlon on the cathode, opposite the crenel on the anode, to decrease the distance between anode and cathode in the crenel part of the device, was necessary to create a stable, periodic domain transit. The device was found to function for range of values between 5.2 to 13.5 microns to 8.5 to 7 microns for a single anode merlon length to crenel length. The optimal ratio was found to be 6.6 to 10.7 microns as shown in figure 3. Note the relative transit lengths in this design are now reversed over the original simple crenellated design. Here the cathode-anode merlon distance is now longer than the cathode-anode crenel distance. In this work the lengths L1 and L2 (figure 1) were varied in the range discussed in section II until the stationary point was found.

Finally, as in [11], it was found that the domains were vulnerable to attraction to any sharp corners on the contacts and this led to undesirable distortion of the domain. Blunting these corners as in [11] reduces this effect and further improved domain behavior.

B. Transit Time mode

Figure 3 shows the domain structure in the diode after four transits of the domain after about 50 ps from the start of the simulation (to allow the device to settle down to steady periodic motion after the initial start-up) under a 2V bias. It can be seen in figure 3 (I) that at 53.2ps the domain has taken on the shape of the cathode. 3.6ps later, figure 3 (II) shows the domain about to make contact with the crenel part of the anode and the current in figure 4 can be seen to be increasing.
The domain passes through the crenel and the current falls until at 60ps when the domain begins to contact the merlon and the current consequently increases for the second peak (figure 3 (III)). Meanwhile the new domain has already formed at the cathode merlon and is in transit whilst the new domain components are forming in the crenel regions of the anode (opposite the merlon regions of the anode). These two parts of the domain will then merge to become one domain again as shown in figure 3 (I).

Figure 4 shows the current output from the device with the steady repeating oscillations with a period of 14ps (70GHz). The fine structure in the peaks, corresponding to the domain boundary, is first incident on the crenel, and then the merlon has a period of 2.8ps (350 GHz), five times greater than the natural period of the transit region length. Potentially the device could be mounted in a high Q circuit and tuned to extract the harmonic (in the above example the fifth harmonic). The output current at the harmonic frequency for these devices will be higher than the output current for a conventional planar Gunn diode therefore offering the potential of THz operation with enhanced output power.

**C. Delayed Domain mode**

For the delayed mode simulations, the optimum structure was found to be $L_1 = 1.30$ and $L_2 = 1.44$ μm. An applied potential with a constant DC component of 2V with a frequency dependent amplitude of 1V at a frequency of 45GHz was found to work well in providing sufficient time to allow the domain to pass through the anode and sufficient change of potential to quench the new domain forming at the anode. Thereby enabling a fresh domain to reform at the cathode as the voltage will again increase above the threshold voltage.

The simulated electron densities during the transit of the Gunn domain in this mode at 47, 50.7, 54.3, 56.8, 62.8 and 65.2 ps are shown in Figures 5 (I-VI) respectively.
each subsequent transit would become greater and the output current waveform progressively more chaotic. However, at this point, the applied potential is about to fall below the threshold voltage for domain formation and the domain is extinguished as shown in figure 5(VI). Finally, when the voltage increases once again, the current increases (62ps in figure 6) and a fresh and relatively straight domain reforms and can be seen in transit within the channel in figure 5(VI) at 65ps.

As can be seen in figure 6, the current waveform shows a lot of fine structure. The prominent peaks at 40 and 63ps correspond to the 45GHz delayed mode potential and the reforming of the domains. The double peaks at 30ps, 52ps and 75ps are each 4ps apart representing the contact of the domain with merlon and then the crenel. This represents a frequency component of 250GHz.

D. Proposed Fabrication Technology

The current semiconductor device fabrication technology is capable of very small feature sizes down to few nm or smaller but some III-V devices such as Field Effect Transistor (FET) and likewise planar Gunn diodes require dimensions longer than several microns for the width but with submicron sized channel gaps. Writing narrow channel gaps between long and wide contacts is difficult by electron beam lithography despite the small beam diameter due to electron beam proximity effects. That is one reason most FET devices with submicron gate lengths are achieved using the gate shadow to deposit the drain and source contact on either side of T-shaped gate. One other possibility could be deposit the gold and then etch small gaps but it is relatively difficult to etch high-resolution gold patterns, and because of this, small gaps between metal contacts are difficult to fabricate using the conventional subtractive processing flow of metal deposition followed by resist patterning and metal etch. Thoms et al [25] previously showed that 100 nm gaps between 100 μm square metal contacts can be realized using a tri-layer of polydimethylglutarimide (PMGI) silicon nitride and UHVIII. The UVIII resist layer is patterned by electron beam lithography. Reactive ion etching (RIE) is used to etch through the silicon nitride layer and a low bias oxygen RIE process is used to etch the sacrificial PMGI layer. The silicon nitride layer is not etched by the plasma and so enables the PMGI layer to be etched back by a controlled amount to give profiles optimal for metal lift off. We have demonstrated the fabrication of planar Gunn diodes using this technique [25-28] down to 100nm channel gaps though we were only able to achieve 600nm channel gap planar Gunn diodes which oscillated. Therefore, we have demonstrable techniques using a combination of several processes to achieve 100nm channels, which will offer the possibility of a low cost and fully integrated THz source.

IV. Conclusion

We have shown it is theoretically possible and experimentally realizable, using shaped anodes and cathodes in a planar Gunn diode to produce stable periodic Gunn domain transits which will yield current waveforms with a fine frequency structure considerably higher in frequency than the nominal transit time of the domain across the channel.

Any shaping of either anode or cathode electrodes can allow distorted domains to develop, with effectively different periods dependent on the travel time between the two shaped contacts making the channel. This distortion can lead to extremely complicated and even chaotic output current waveforms. However, by careful choice of the widths of the channel, it is possible to achieve stable operation by two methods: by utilizing the property of negative differential resistivity to find points of stationary time of transit, despite small differences in transit region length and by using delayed mode oscillations in which the Gunn domains are quenched after each transit forming anew with no memory of previous transits.

As mentioned in the introduction, so far, the RF output power and efficiency of the standard Planar Gunn diode with the straight edged anode and cathode electrodes has been disappointing. The prospects for a reasonable amount of power extraction in a fifth harmonic might at first sight therefore not look very good with the existing research devices produced so far. Theoretical calculations, however, have shown the output power and efficiency should be at least comparable to the vertical Gunn diodes and a recent theoretical work [11] has shown by improving the planar Gunn diode electrode geometry, enhanced domain propagation can be obtained leading to the potential of substantial improvements in both RF output power and efficiency. In addition, the planar Gunn diode concept has the potential to be fully integrated into MMIC technology and offers the prospect of adding multiple devices to improve power and efficiency. Normally, in Gunn diode systems, only the second or third harmonic is chosen as a practical power source since higher harmonics will produce an almost unusable RF output power. However, the current research work indicates that these devices are actually generating current output at this harmonic and this suggests the potential for useful power generation is a real possibility in chip based terahertz systems that would be mass producible. The power efficiency may still remain low but with multiple integrated devices a reasonable power generation is a real prospect. It is also interesting to note that, the ability to shape waveforms by sculpturing the anode and cathode may have other interesting waveform shaping applications.
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REFERENCES