# Monte Carlo-Based Harmonic-Balance Technique for the Simulation of High-Frequency TED Oscillators

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***Abstract*— A harmonic-balance technique for the analysis of high-frequency transferred electron device (TED) oscillators is developed. The behavior of the nonlinear TED is not obtained from a quasi-static equivalent circuit; rather, a physical transport model is used to determine its response in time domain. This model is based on the ensemble Monte Carlo technique coupled to a heat-flow equation, which accounts for thermal effects on the device operation. It is found that the standard splitting method for updating the unknown voltage across the diode fails to converge to a steady-state solution at the fundamental frequency. A modified version is proposed, which updates the voltage at the fundamental and higher harmonics differently. This method exhibits much better convergence behavior. Simulation results obtained with the complete model are in very good agreement with experimental data from InP TED oscillators operating at 131.7 and 151 GHz in the fundamental mode and at 188 GHz in the second-harmonic mode.**

***Index Terms*—Harmonic balance, Monte Carlo, semiconductor device modeling, transferred electron devices.**

## I. Introduction

TOWARD THE development of sources of power generation at frequencies above 100 GHz, InP transferred electron devices (TED's) have shown great promise in meeting this challenge. In particular, significant output power levels have been realized over much of the $D$-band (110–170 GHz) frequency region from InP TED's operating in the fundamental mode [1], [2]. Further improvement in oscillator performance could be realized by TED structures that incorporate a heterojunction injector at the cathode [3]. However, at some point, a frequency limit is reached for fundamental-mode operation, and harmonic generation should be considered. Extraction of RF power at higher harmonics would enable InP TED's to cover the millimeter-wave and part of the submillimeter-wave regions.

This paper addresses issues related to the modeling of InP TED oscillators operating at these high frequencies. In general, the modeling task involves a description of the device operation and its interaction with the external circuit. InP TED operation is strongly nonlinear and is not easily amenable to analytical formulation. Therefore, it is common to resort to a computer model based on the physics of the Gunn effect. Three transport models are widely used:

1) drift-diffusion;
2) energy-momentum;
3) Monte Carlo.

The first two are derived from the Boltzmann transport equation and consist of a set of differential equations representing balance of average carrier energy, average carrier momentum, and carrier density. The Monte Carlo approach is different in that it mimics the transport dynamics of individual carriers subject to internal and external forces and the various scattering mechanisms. The assumptions underlying the drift-diffusion model limit its validity to devices with few microns in size and under conditions of slowly varying electric fields in time and space [4]. The energy-momentum model does not suffer from these limitations; however, it requires the specification of energy and momentum relaxation times, which depend on the carrier energy and represent the effect of the scattering processes on the carrier transport. In modeling the effect of all scattering phenomena by few relaxation-time parameters, some of the physics would necessarily be lost. In particular, for TED devices, the Gunn effect is strongly related to the scattering processes between various conduction-band valleys. Therefore, it is important to accurately take into account this type of scattering, especially at the high frequencies of interest in this paper. The Monte Carlo model provides such a description and will be used to simulate the TED behavior subject to an applied voltage.

TED's are characterized by a negative resistance at some frequency band determined mainly by its size, doping, and mode of operation. When placed in a resonant circuit, well-defined oscillations can be established, and RF power can be extracted. The interaction between the TED device and the resonant circuit is generally described either by assuming that steady-state oscillations have been established and the diode is driven by a known RF voltage, or the evolution of the diode and the resonant circuit is simulated starting from an initial noise signal until stable oscillations are established. This paper reports on an implementation of the second method, whereby the resonant circuit is described by a set of load impedances at the fundamental and higher harmonic frequencies, and the diode behavior is simulated in the time domain with a self-consistent ensemble Monte Carlo model. To establish the operating point of the TED oscillator, an arbitrary initial voltage is assumed across the diode at all frequencies of inter-

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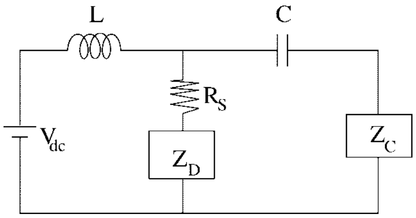


Fig. 1. Equivalent circuit of the TED oscillator.

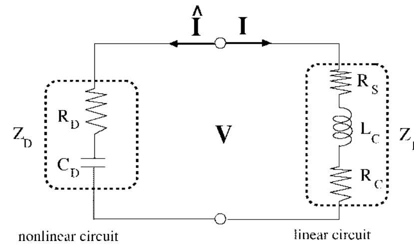


Fig. 2. Partitioning of the TED oscillator circuit into linear and nonlinear subcircuits.

est, and the harmonic-balance technique is used to iteratively update the voltage until the current into the diode is consistent with the current into the embedding circuit. A procedure based on the splitting method has been adopted for updating the unknown voltage. It is found that the standard splitting method fails to yield a stable solution. A modified splitting method is proposed where the voltage component at the fundamental frequency is updated differently from components at higher harmonics. The new method converges to a stable solution for the TED oscillator circuit. Application of the Monte Carlo-based harmonic-balance technique to the simulation of InP TED's will be presented, and the results will be compared with available experimental data.

## II. TED OSCILLLATOR

A TED device in a resonator can be represented by the equivalent circuit shown in Fig. 1. $Z_D$ is the Gunn-diode equivalent impedance, $Z_C$ is the circuit equivalent impedance (as seen at the diode terminals), and $R_S$ is the series resistance, which is frequency dependent and represents losses due to substrate, skin effect, and contact resistances. The inductor $L$ isolates the dc voltage from the RF signal, whereas the capacitor $C$ is assumed large enough to behave as a short at frequencies of interest while preventing any dc current through $Z_C$. Under dc conditions, the voltage across the diode is $V_{\rm dc}$ less the voltage drop across the series resistance $R_S$. The impedances $Z_D$ and $Z_C$ can be expressed as

$$Z_D = R_D + jX_D \tag{1}$$

and

$$Z_C = R_C + jX_C. \tag{2}$$

The oscillation condition requires that $Z_D + Z_C + R_S = 0$ at the fundamental frequency and higher harmonics. This condition translates into the following two equations:

$$R_D(f, V, T) + R_C(f) + R_S(f) = 0 \tag{3}$$

and

$$X_D(f, V, T) + X_C(f) = 0. \tag{4}$$

In general, the objective of simulating a TED oscillator is to estimate the output power and conversion efficiency at a particular frequency of interest. Although the circuit shown in Fig. 1 is relatively simple, accurate analysis is not a straightforward task. This is mainly due to the fact that the TED is a nonlinear device. For example, the diode's equivalent impedance $Z_D$ depends in a complex nonlinear fashion on frequency, voltage across the diode, and the operating temperature. Such dependence cannot be easily described by analytical formulas and has to be determined by means of a complete simulation of the electron transport dynamics. Such simulation has to accurately depict the physical phenomena relevant to the Gunn effect. A model based on the ensemble Monte Carlo technique has been developed for the simulation of TED structures in various material systems and for different cathode-injection mechanisms. Results obtained with this model were in very good agreement with experimental data [1]. In the original implementation, the dc voltage, RF voltage at the fundamental frequency, and load resistance were specified as input parameters. The simulation provides the current response in the time domain from which the diode equivalent impedance, output RF power, conversion efficiency, and required diode area for matching the load could be determined at the fundamental frequency. To estimate the maximum output power, many simulation runs need to be performed with various RF voltage levels. Instead, it is desirable to specify the dc voltage, operating frequency, device area, and load impedance, and perform the simulation to determine the voltage and current across the diode which fulfill the oscillation condition. In this paper, we present an implementation of such a method based on the harmonic-balance technique coupled to the ensemble Monte Carlo technique for semiconductor device modeling. In addition, the new implementation is well suited for the analysis of TED oscillations for power generation at the second harmonic and higher.

## III. HARMONIC-BALANCE METHOD

The harmonic-balance technique is widely used to analyze strongly nonlinear circuits. In this method, the circuit is divided into a subcircuit consisting of linear elements and a subcircuit containing nonlinear elements, e.g., active semiconductor devices. It then searches for a voltage waveform at the various ports in the circuit such that the current flowing into the linear subcircuit is consistent with the current flowing into the nonlinear subcircuit. The TED oscillator circuit is redrawn in Fig. 2 to illustrate the two subcircuits. The diode series resistance $R_S$ is combined within the circuit impedance $Z_C$ to form the impedance of the linear subcircuit $Z_L = R_L + jX_L$. This is equivalent to the original circuit in Fig. 1 at the high frequencies of interest. The TED diode represents the nonlinear element, whereas the resonant circuit and any series resistances represent the linear subcircuit. Denoting the common voltage across the diode and linear circuit by $\mathbf{V}$, the current into the diode $\hat{\mathbf{I}}$ should then be equal in amplitude to the current into the linear circuit $\mathbf{I}$ under steady-state conditions. At the fundamental frequency, it is assumed that the resonant circuit can provide the necessary reactance to cancel the diode's reactance $X_D$ according to condition 4. The simulation task consists of finding the voltage across the diode such that

$$f(\mathbf{V}) = \mathbf{I} + \hat{\mathbf{I}} = 0 \tag{5}$$

where $\mathbf{V}$, $\mathbf{I}$, and $\hat{\mathbf{I}}$ are one-dimensional vectors consisting of the Fourier transform of $v(t)$, $i(t)$, and $\hat{i}(t)$:

$$\begin{aligned}\mathbf{V} &= [V_1 \quad V_2 \quad \cdots \quad V_K]\\ \mathbf{I} &= [I_1 \quad I_2 \quad \cdots \quad I_K]\\ \hat{\mathbf{I}} &= [\hat{I}_1 \quad \hat{I}_2 \quad \cdots \quad \hat{I}_K]\end{aligned} \tag{6}$$

where $K$ is the number of harmonics included. The terms corresponding to $V_0$, $I_0$, and $\hat{I}_0$ are not included since the capacitor blocks any dc signal to the linear circuit. The dc voltage is specified as an input parameter which is kept constant for the duration of the simulation. At any point in time, the total voltage across the diode corresponds to the sum of a dc-voltage term and RF components at the fundamental frequency and higher harmonics. The dc voltage consists of $V_{\mathrm{dc}}$ less the voltage drop across the series resistance $R_S$. Clearly, one solution to (5) corresponds to $\mathbf{V} = 0$, which is of no interest here. A solution different from zero is possible only if $R_D$ is negative, which can be provided by the TED when properly designed and biased. There are many techniques for solving the nonlinear equation (5), including Newton's method, splitting method, optimization, and reflection algorithm [5].

In this paper, we consider a modified splitting method, which is an iterative technique for updating the solution. Given an estimate of the unknown voltage at the $n$th iteration $\mathbf{V}^n$, a new estimate is obtained according to the following procedure. The current $\hat{\mathbf{I}}$ flowing into the diode is computed. This generally requires one to analyze the diode in time domain by performing a simulation of carrier transport for at least one period. The current into the linear subcircuit is assumed to be equal in amplitude to the current obtained from the nonlinear circuit, i.e., $\mathbf{I} = -\hat{\mathbf{I}}$. A new voltage $\mathbf{V}''$ across the linear circuit is then calculated as

$$\mathbf{V}'' = \mathbf{Z}_L \mathbf{I} = -\mathbf{Z}_L \hat{\mathbf{I}}. \tag{7}$$

where $\mathbf{Z}_L$ is a diagonal matrix with entries corresponding to the various harmonic frequencies. A new estimate of the voltage $\mathbf{V}^{n+1}$ at the $(n+1)$th iteration, geometrically between $\mathbf{V}^n$ and $\mathbf{V}''$, is generated:

$$\mathbf{V}^{n+1} = \alpha \mathbf{V}'' + (1-\alpha)\mathbf{V}^n \tag{8}$$

where $\alpha$ is a real constant between 0–1 and is referred to as the splitting parameter. The above procedure is repeated until $f(\mathbf{V})$ approaches zero to within the desired tolerance. Let us define a "quasi-impedance" $\mathbf{Z}_D$ of the Gunn diode as a diagonal matrix with entries given by [6]

$$Z_D(k\omega_0) = \frac{V(k\omega_0)}{\hat{I}(k\omega_0)} = \frac{1}{Y_D(k\omega_0)}, \qquad k = 1, 2, \cdots, K \tag{9}$$

where $\omega_0$ is the fundamental frequency. Substituting $\hat{\mathbf{I}}$ by $\mathbf{Y}_D\mathbf{V}^n$, (8) can be rewritten as

$$\mathbf{V}^{n+1} = \alpha \mathbf{Z}_L(-\mathbf{Y}_D\mathbf{V}^n) + (1-\alpha)\mathbf{V}^n \tag{10}$$

or

$$\mathbf{V}^{n+1} = [(1-\alpha)\mathbf{I} - \alpha \mathbf{Y}_D \mathbf{Z}_L]\mathbf{V}^n \tag{11}$$

where $\mathbf{I}$ is the identity matrix. In the standard splitting method for updating the solution, the parameter $\alpha$ takes real values between 0–1. Under this condition and using (1) and (2), the component of (11) corresponding to the fundamental frequency is written as

$$V_1^{n+1} = \left[\frac{1 + \alpha(\beta - 1) + j\,\dfrac{X_D}{R_D}}{1 + j\,\dfrac{X_D}{R_D}}\right] V_1^n. \tag{12}$$

In the last equation, $X_L$ has been expressed as $-X_D$ and $R_L$ as $\beta|R_D|$ where $\beta$ is a positive real number and $R_D$ is negative. There are two cases for $\beta$:

*Case 1)* $0 < \beta < 1$ corresponding to $R_L < |R_D|$. This implies that $1 + \alpha(\beta - 1) < 1$ and, therefore, $|V_1^{n+1}| < |V_1^n|$.

*Case 2)* $\beta > 1$ corresponding to $R_L > |R_D|$. This implies that $1 + \alpha(\beta - 1) > 1$ and, therefore, $|V_1^{n+1}| > |V_1^n|$.

However, because the TED equivalent resistance $|R_D|$ tends to decrease as the amplitude of the voltage across the diode is increased, such a scheme for updating $V^n$ would result in widening the difference between $R_L$ and $|R_D|$ and moving further away from the solution satisfying the oscillation condition. To overcome this problem, a modified splitting method is proposed, where $\alpha$ is assigned negative real values at the fundamental frequency and positive values at the higher harmonics. In such a scheme, the relation between $\mathbf{V}^{n+1}$ and $\mathbf{V}^n$ on a component-by-component basis is as follows:

$$\begin{aligned}V_1^{n+1} &= \left(\frac{1 - \alpha_1 - \alpha_1 Z_L(\omega_0)}{Z_D(\omega_0)}\right) \qquad V_1^n\\ V_2^{n+1} &= \left(\frac{1 - \alpha_2 - \alpha_2 Z_L(2\omega_0)}{Z_D(2\omega_0)}\right) \qquad V_2^n\\ &\vdots\\ V_K^{n+1} &= \left(\frac{1 - \alpha_K - \alpha_K Z_L(K\omega_0)}{Z_D(K\omega_0)}\right) \qquad V_K^n\end{aligned} \tag{13}$$

where $\alpha_k$ is negative for $k = 1$ and positive for $k = 2, \cdots, K$.

## IV. Harmonic-Balance and Monte Carlo Methods

The self-consistent-ensemble Monte Carlo model is used to characterize the electron transport in TED devices. At frequencies above 100 GHz, the Monte Carlo method is more appropriate than other models based on solving balance equations derived from the Boltzmann transport equation. In particular, for the TED effect, the Monte Carlo method allows the consideration of various scattering mechanisms individually rather than through average relaxation times. The ensemble Monte Carlo model is an extension of the one-particle Monte Carlo technique [7]. It describes the transport process in a TED structure by simulating a group of electrons simultaneously. The electric field is to be updated regularly since it is evolving as the electrons redistribute themselves in the device. The analysis is carried out assuming the device behavior is mainly one-dimensional, which is justified for two terminal devices. A diode structure of length $L$ is divided into cells of equal length ($\Delta x = 50$ Å). Any attributes of the electrons are averaged over each cell and assigned to the midway position of the cell. The cell size should be smaller than the smallest Debye length in the structure, which occurs at the highly doped regions.

The simulation algorithm consists of monitoring the evolution in real and momentum spaces of an ensemble of electrons. The simulation time is partitioned into time steps ($\Delta t = 5 \times 10^{-15}$ s), and each time step is terminated by a call to a Poisson-equation solver in order to update the electric field. In each time step, every electron is submitted to successive free flights terminated by a scattering process, which is selected using a random-number generator. Electrons crossing cell boundaries are temporarily stopped at that boundary and then resumed with the electric field in the new cell. An analogous procedure is followed when it is time to update the electric field and the electron is in the middle of a free flight. In this case, the remaining flight time is stored and the flight is resumed after all other electrons are simulated for one time step, the carrier density is calculated, and the electric field is updated.

The remainder of this section discusses how the performance of a TED oscillator (output power and efficiency) is estimated using the Monte Carlo program. It also describes the procedure for coupling the Monte Carlo program to the harmonic-balance technique. The Monte Carlo simulation proceeds by distributing an ensemble of electrons ranging from 10 000 to 20 000 among the cells in the device. The number of electrons assigned to each cell is proportional to the doping level in that cell. Initially, the electric field is assumed uniform in space with a value determined by the applied dc voltage and the length of the device. It is noted that the initial electron distribution and electric-field profile influence the transport only for the first few RF periods. Thereafter, the results of the simulation are independent of this choice. Each electron is followed for a time step $\Delta t$ subject to the local electric field and the various scattering mechanisms. Whenever an electron leaves one of device terminals, it is injected back into the device with a drifted Maxwellian distribution. At the end of $\Delta t$, the electron density and average current across the device are computed. With the new density, the electric field is updated by solving Poisson's equation. This procedure is repeated until a desired number of RF periods is reached. As a result of the simulation, abundant information about the device operation can be extracted. For instance, the average electron velocity, energy, and distribution in the various conduction-band valleys could be easily obtained as a function of time and position along the device.

An important feature was added to the Monte Carlo program to enhance the accuracy of the simulation results obtained. It consists of incorporating thermal effects on the device operation. It is known that TED's used for power generation operate at a much higher temperature than the ambient temperature. This is due to the relatively low conversion efficiencies at high frequencies. It is important to incorporate thermal effects in the simulation because the electron transport and, as a result, the current response and output power are very sensitive to the device operating temperature. This is achieved by coupling a heat-flow equation to the Monte Carlo model. The heat generation density across the device is determined by considering the energy exchange between the electric field, electron, and lattice systems. Specifically, it is obtained from the net phonon energy exchange between the lattice and the electron system. It is then used to solve the heat-flow equation for the lattice temperature profile. The new temperature across the device influences the dynamics of electron transport through modified scattering rates. The transport problem and the heat-flow equation are solved until a consistent lattice temperature solution is reached. The Monte Carlo model coupled to the heat-flow equation was used to simulate a TED oscillator with copper and diamond heat sinks. Good agreement was obtained between the simulation and experimental results [8].

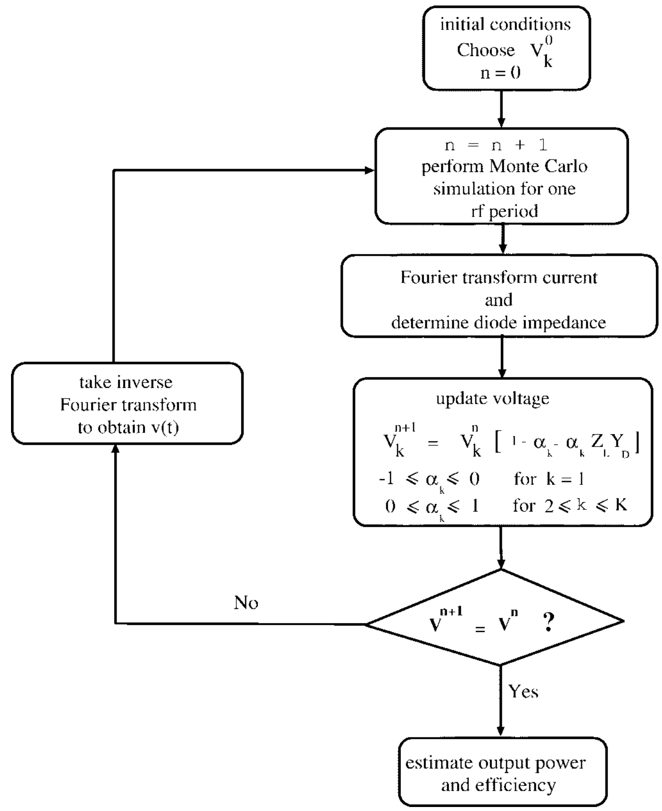


Fig. 3. Procedure for coupling the harmonic-balance and Monte Carlo techniques.

In coupling the Monte Carlo method to the harmonic-balance technique, the RF voltage across the device is not specified as an input parameter. Rather, it is initially chosen arbitrarily small, which represents the noise signal in a real oscillator. The new model is represented by the flowchart shown in Fig. 3. It starts by specifying the initial conditions

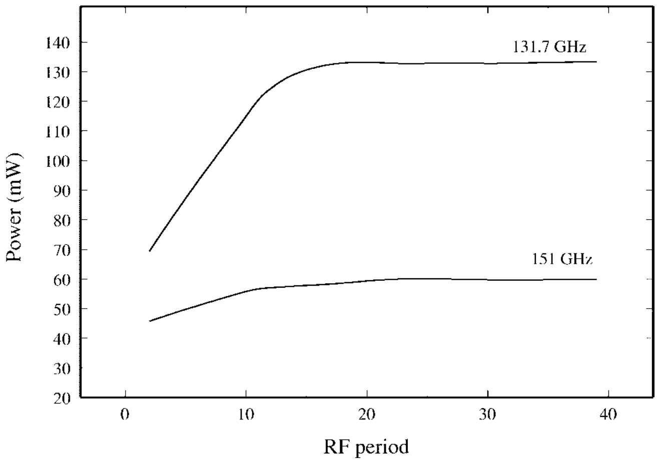


Fig. 4. Simulation results showing the output RF power at the fundamental frequency from an InP device with a graded doping profile in the active region. The power is plotted at each RF simulation period for two oscillation frequencies of 131.7 and 151 GHz.

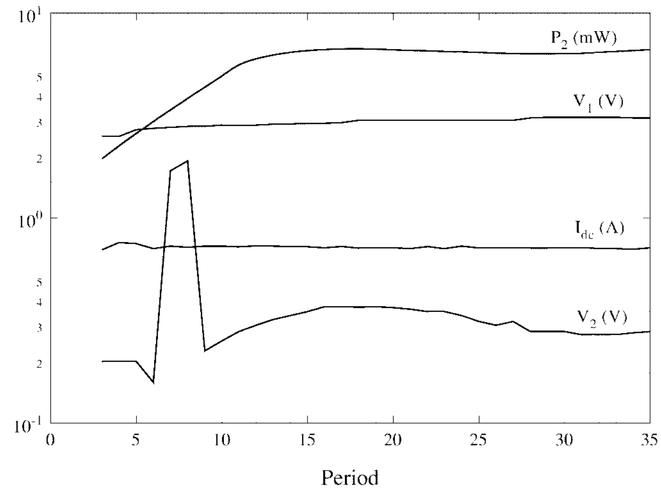


Fig. 5. Simulation results of the output power at the second harmonic, voltage amplitude at the fundamental frequency $V_1$ and second harmonic $V_2$, and dc current $I_{\rm dc}$ at various periods.

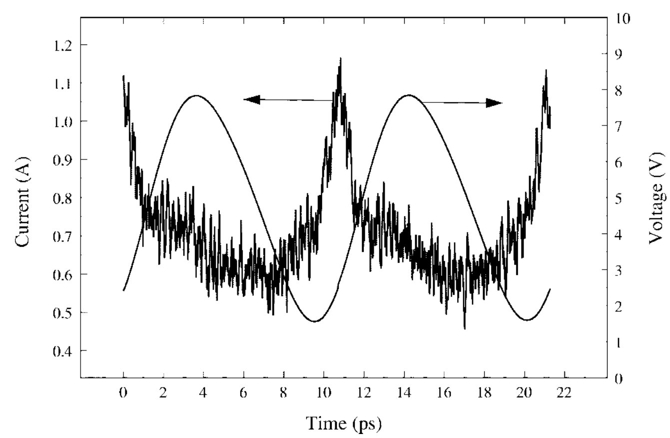


Fig. 6. Final solution of the total current and voltage waveforms across the TED diode.

which define the device structure and size, fundamental frequency of operation, load impedance, and dc-bias voltage. A Monte Carlo simulation of the electron transport, as described above, is then performed for one RF period corresponding to the fundamental frequency. The resulting current response in time domain is Fourier transformed and the device quasi-impedance $Z_D$ is computed based on (9). At this point, the voltage across the diode is updated according to (13) with $\alpha_1 = -1$ for the fundamental component $V_1$ and $0 < \alpha_k < 1$ for the higher harmonics $V_k$, $k > 1$. The total voltage across the device is adjusted to correspond to the new RF voltage and dc bias. The new voltage is compared with the value in the previous period. In case the difference is still large, the inverse Fourier transform of the voltage is performed and the Monte Carlo simulation is repeated for another period. In general, it is found that a stable solution is reached within 40 RF periods.

## V. Comparison with Experiment

In order to evaluate the accuracy of the Monte Carlo-based harmonic-balance model, simulation results should be compared with available experimental data. For the case of $K = 1$, which corresponds to fundamental-mode operation, the model predictions are compared with experimental results obtained from an InP TED structure with a graded doping profile in the active region. Specifically, it consists of a 1-$\mu$m-long active region with n-type doping increasing from $7.5 \times 10^{15}$ cm$^{-3}$ at the cathode to $2.0 \times 10^{16}$ cm$^{-3}$ at the anode side [1]. Experimentally, devices with this structure yielded 130 mW at 131.7 GHz and 60 mW at 151 GHz [2]. Simulations were performed on a similar structure mounted on a diamond heat sink. The predicted output RF power as a function of the RF simulation period is shown in Fig. 4 at two oscillation frequencies of 131.7 and 151 GHz. Clearly, our model provides good agreement with the measured data.

For the case of $K = 2$, which corresponds to the second harmonic operation, fewer experimental results are available at frequencies above 180 GHz. Rydberg [9] has reported experimental results on harmonic-power generation from InP TED's. The tested devices were based on a structure described in [10]. It consists of a 1–1.1-$\mu$m active region with a doping in the $1.5 \times 10^{16}$ cm$^{-3}$ to $2 \times 10^{16}$ cm$^{-3}$ range and 40–60 $\mu$m in diameter. Second harmonic power levels up to 7 mW were observed at frequencies between 180–190 GHz from devices biased at a dc voltage of 4.8 V and with a dc current of approximately 700 mA. For the purpose of comparing these results with the harmonic-balance simulation, a 1.1-$\mu$m structure is considered with a doping of $1.5 \times 10^{16}$ cm$^{-3}$ and a dc voltage of 4.8 V. Simulations were performed at a fundamental frequency of 94 GHz for 35 periods with a splitting parameter of $-1$ at the fundamental frequency and 0.5 at the second harmonic. At 94 GHz, the simulation predicts an output power of 70 mW and a dc current of 710 mA in agreement with the experimental results provided by Rydberg. Fig. 5 shows the evolution of the output power at the second harmonic (188 GHz), voltage amplitude at the fundamental $V_1$, voltage amplitude at the second harmonic $V_2$, and dc current during the simulation. About 6.5 mW is predicted at 188 GHz with $V_1 = 3.0$ V and $V_2 = 0.3$ V. These results are to be compared with a measured output power between 5–6 mW at 188 GHz. Fig. 6 shows the final solution for

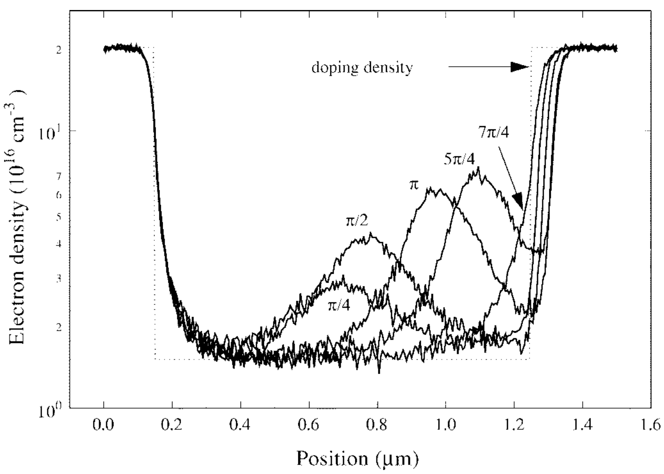


Fig. 7. Snapshots of the electron density at various points in one RF period illustrating the growth and drift of accumulation layers.

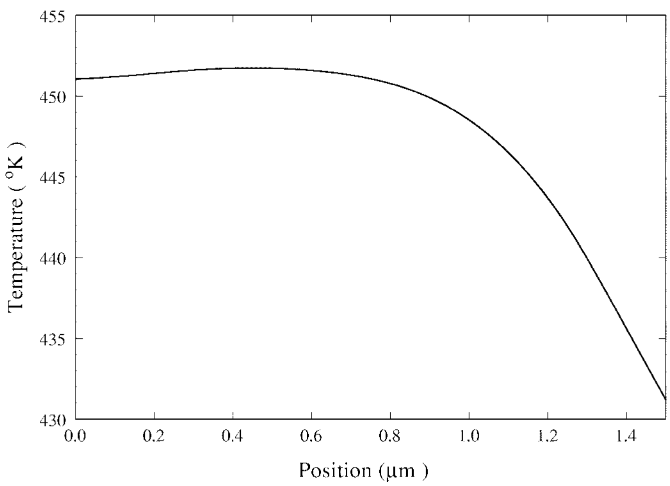


Fig. 8. Steady-state operating temperature profile along the TED structure. The heat sink is located at a position of 1.45 $\mu$m.

the total voltage and current waveforms across the diode. The current oscillations correspond to the formation of space charge accumulation layers. This is illustrated in Fig. 7, which shows the doping density and electron density at various points in one RF period.

In addition to updating the voltage across the diode at the end of each period according to the harmonic-balance method, the temperature across the device is also updated by solving the heat-flow equation. Fig. 8 shows the steady-state temperature profile across the TED diode. The temperature increases from 431 K at the anode region where the copper heat sink is located to 451 K at the cathode region.

## VI. Conclusion

This paper reports on the development of a computer model for the simulation of high-frequency TED oscillators. It is based on the harmonic-balance technique, where the nonlinear behavior of the TED is modeled according to the ensemble Monte Carlo approach to semiconductor device simulation. Starting from a small voltage signal, the model predicts the steady-state device operating conditions such as the large-signal current and voltage waveforms, temperature profile across the diode, and output power at the fundamental and higher harmonics. It is found that the standard splitting method for updating the unknown voltage across the diode fails to converge to a stable solution. A new approach is proposed where the splitting parameter is assigned negative real values for updating the voltage at the fundamental frequency and positive real values at higher harmonics. Large-signal results obtained with this model are in excellent agreement with experimental data from an InP TED oscillator operating at a fundamental frequency of 94 GHz.

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