Electrical and Thermal Phenomena Simulation of Pulsed-Mode IMPATT Diode

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Abstract: - The problem of the adequate analysis of some semiconductor structure can be solved on the base of numerical nonlinear complex model. A numerical model that includes electrical and thermal sub models was developed for the analysis of various IMPATT-generator operation modes. Electrical model is based on the system of continuity equations for a semiconductor structure.

Data on the temperature distribution that is necessary for the calculation of the local-field electrical model are obtained from IMPATT-diode thermal model. This thermal model determines the temperature distribution in all points of the diodes active layer, for any given moment in time. The IMPATT-diode thermal model is based on the numerical solution of the non-linear thermal conductivity equation for silicon crystal, contact planes and heat sinks. It is very important to obtain the solution of this equation with great accuracy for minimum computer time because as a rule this equation is only one part of more complicated problem for the analysis and optimization of a microwave semiconductor device. In this work this problem has been successfully solved on the base of the high-order numerical scheme for heat conductivity equation. On the base of the forth order numerical scheme for Laplace operator approximation, numerical algorithm for the thermal conductivity equation solution is developed. In that case we can use the numerical net that is more thin significantly for the obtaining accuracy that is equal to the ordinary scheme of second order approximation. This method was successfully used jointly with the electrical model of semiconductor structure.

Analysis and internal structure optimization of the pulsed-mode silicon IMPATT diode for different frequency regions shows a perspective of this complex model.

Key Words: - Microwave semiconductor devices, modeling and simulation, numerical methods.
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1 Introduction

IMPATT diode is the principal active element for use in millimetric pulsed-mode generators. Semiconductor structures suitable for fabrication of continuos-mode IMPATT diodes have been well known for a long time [1-2]. They have been utilized successfully in many applications in microwave engineering. The possibilities of using the same structures for pulsed-mode microwave generators are very interesting because the pulsed-mode IMPATT-diode generators can successfully operate at high current densities without deterioration of reliability. The cross section of the pulsed-mode IMPATT diode may be larger than that of the continuous-mode diodes. Therefore, the pulsed-mode oscillator can provide a larger power output. Considering, that the increase of the output power of millimetric generators is one of the main problems of microwave electronics; it is important to optimize the diode active layer to obtain the generator maximum power output.

One of the main singularities in the operation of high-power IMPATT-diode pulsed-mode generator, is the large variation of the diode admittance during the pulse. This variation is significantly during each current pulse due to the temperature changing of the diode semiconductor structure. Therefore, diffusion coefficients, ionization rates and charge mobility experience large variations during the pulse. These changes strongly affect the amplitude and phase of the first harmonic of the diode avalanche current. Therefore, the admittance value also changes. This results in the instability of generator output power and frequency within each generated microwave pulse.

Pulsed-mode IMPATT diodes that are utilized in microwave electronics are, most frequently, the single-drift and double-drift structures similar to continuous-mode ones [1-3]. The typical diode structure is shown in Fig. 1 by curve 1, where N is the concentration of donors and acceptors, l is the length of diode active layer. In this type of diodes, the electrical field is strongly distorted when the avalanche current density is sufficiently high. This large space charge density is one of the main reasons for the sharp electrical field gradient along the charge drift path. Because of this field gradient, the space charge avalanche ruins itself and consequently the optimum phase relations degrade between microwave potential and current. This factor is especially important when the IMPATT diode is fed at the maximum current density, which is exactly the case at the pulsed-mode operation.

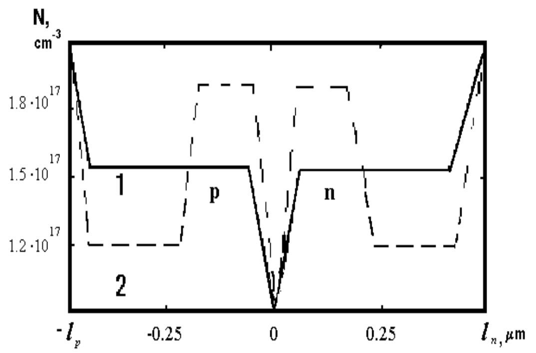

Fig.1 Doping profile for two types of IMPATT diodes:
1 - even doping profile; 2 - complex doping profile.

The idea to utilize a complex doping profile semiconductor structure for microwave diode was originally proposed in the first analysis of IMPATT diode by Read [4]. This proposed ideal structure has never been realized till now. However, a modern semiconductor technology provides new possibilities for the fabrication of sub micron semiconductor structures with complex doping profiles. This stimulates the search for IMPATT-diode special structure optimization for pulsed-mode operation.

The proposed new type of IMPATT diode doping profile is shown in Fig. 1 by the curve 2. This type of semiconductor structure can be named as quasi-Read-type structure. This type of doping profile provides a concentration of electrical field within the *p-n* junction. This measure helps to decrease the destruction of the avalanche space charge and therefore permits to improve the phase stability between the diode current and voltage.

Historically, many analytical and numerical models have been developed for the various operational modes of IMPATT diodes [1-7]. However, they are not adequate for very high current density values and different temperature distributions inside the structure, which is exactly the case for the pulsed-mode IMPATT-diode oscillator. For this reason, we have developed a new complex numerical model of the IMPATT diode that is composed of the advanced thermal model and the modified local-field model.

2 Numerical model

The complex numerical model is developed for the analysis of various generator operation modes. This model includes electrical and thermal sub models.

2.1 Electrical model

This model is based on the system of continuity equations for semiconductor structure:

$$\frac{\partial n(x,t)}{\partial t} = \frac{\partial J_n(x,t)}{\partial x} + \alpha_n \left|J_n(x,t)\right| + \alpha_p \left|J_p(x,t)\right|$$

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J_p(x,t)}{\partial x} + \alpha_n \left|J_n(x,t)\right| + \alpha_p \left|J_p(x,t)\right| \qquad (1)$$

$$J_n(x,t) = n(x,t)\, V_n + D_n \frac{\partial n(x,t)}{\partial x}$$

$$J_p(x,t) = p(x,t)\, V_p - D_p \frac{\partial p(x,t)}{\partial x}$$

where n, p are concentrations of electrons and holes; J_n, J_p are current densities; α_n, α_p are the ionization coefficients; V_n, V_p are drift velocities; D_n, D_p are diffusion coefficients. Ionization coefficients, drift velocities and diffusion coefficients are functions of two arguments, x and t.

This model is differs from the previously proposed models, described in [3-7] because in the present model the ionization coefficients are functions of electric field and temperature at all points of semiconductor structure. The dependence of these coefficients on temperature can be approximated using the approach described in [8].

Boundary conditions for this system are given by:

$$n(0,t) = N_D(0); \qquad p(l_0,t) = N_A(l_0);$$
$$J_n(l_0,t) = J_{ns}; \qquad J_p(0,t) = J_{ps}. \tag{2}$$

where J_{ns}, J_{ps} are the electron current and hole current for inversely biased *p-n* junction; $N_D(0)$, $N_A(l_0)$ are the concentrations of donors and acceptors at two space points x = 0 and x = l_0; l_0 is the length of the active layer of semiconductor structure.

Electrical field distribution into semiconductor structure can be obtained from Poisson equation. As electron and hole concentrations are functions of the time, therefore, this equation is time dependent too and time is the equation parameter. Poisson equation for this problem has the following form:

$$\frac{\partial E(x,t)}{\partial x} = -\frac{\partial^2 U(x,t)}{\partial x^2} = N_D(x) - N_A(x) + p(x,t) - n(x,t)$$

where $N_D(x)$, $N_A(x)$ are concentration of donors and acceptors accordingly, *U(x,t)* is the potential, *E(x,t)* is the electrical field.

These equations adequately describe processes in IMPATT diode in a wide frequency band. However, numerical solution of this system of equations is very difficult because of the existing sharp dependence of equation coefficients on electric field. Evident numerical schemes have poor stability and require a lot of computer time for a good calculation accuracy obtaining. It is more advantageous to use non-evident numerical scheme, that has a significant property of absolute stability.

After the approximation of functions and its differentials, the system (1) is transformed to the non-evident modified Crank-Nicolson numerical scheme.

The approximation of the Poisson equation is performed using the ordinary finite difference scheme at every time step k:

$$U_{i-1}^k - 2U_i^k + U_{i+1}^k = h^2\left(N_{Di} - N_{Ai} + p_i^k - n_i^k\right)$$

The total algorithm for the calculation of IMPATT diode characteristics consists of the consecutive steps for the principle numerical equations' solution. This process is continued until the convergence is achieved. The current in external electronic circuit is determined and then by the Fourier transformation all harmonics of external current, admittance, and power characteristics can be calculated.

2.2 Thermal model

Data on the temperature distribution that is necessary for the calculation of the local-field electrical model may be obtained from IMPATT diode thermal model. This thermal model allows the determination of the thermal conditions in all points of the diodes active layer, for any given moment in time.

The IMPATT diode thermal model is based on the numerical solution of the non-linear thermal conductivity equation for silicon crystal, contact planes and heat sinks. It determines the instantaneous semiconductor structure temperature at any point within the device for any "long" time moment t'. This equation is solved in the region that is shown in Fig.2.

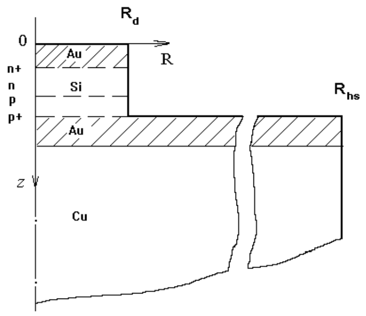

Fig. 2 The schematic diode construction with heat sink. R_d is the diode radius, R_{hs} is the heat sink radius.

The thermal equation has the following form:

$$\frac{\partial T}{\partial t'} = \frac{k}{\rho C}\left\{\frac{\partial^2 T}{\partial x^2} + \frac{\partial}{\partial R}\left(R\frac{\partial T}{\partial R}\right)\right\} + \frac{1}{\rho C}\overline{Q}\,(x,t',T) \tag{3}$$

where t' is the time coordinate (this time scale differs from the scale in the system (1)); R is the radial coordinate; x is the longitudinal coordinate; T is the Kelvin temperature; ρ is the material density ; C is the specific thermal capacity; k is the thermal conductivity coefficient; $\overline{Q}\,(x,t',T)$ is the average for

the high frequency period value of internal heat source. This equation is solved within a volume that includes the silicon crystal; the gold contact plane deposited on the crystal; an integrated thermal contact and the semi-infinite copper heat-sink. For this equation, the boundary conditions are follows:
$\frac{¶\ T}{¶\ r} = 0$ on the vertical axis of symmetry; $\frac{¶ T}{¶ r} = -l(T-q)$ on all vertical boundaries facing the air; $\frac{¶\ T}{¶\ x} = -l\ (T-q)$ on all horizontal boundaries facing the air; $\frac{¶\ T}{¶\ x} = -\frac{q(t')}{k}$ on the internal boundary with a semi-infinite copper heat sink. The variable l is the heat transmission coefficient on the metal-air boundary; q is the air temperature; $q(t')$ is the thermal flux entering semi-infinite copper heat sink.

The principal difference between the equation (3) and the system (1) is that: in (3), function T depends on two spaces coordinates x and R. Contrary to this, in the system (1), all functions depend only on one space coordinate, x. The dependence of all functions of system (1) on R can be neglected, because of approximations which result in negligible error. However, the same dependence can not neglect for equation (3), because it corresponds to the two-dimensional case (Fig. 2).

The process of elaboration of the IMPATT-diode thermal model includes the determination of the functional dependence of the internal heat source $\overline{Q}(x,t',T)$ on the temperature. The model may be simplified by the following important approximations: the role of some metal layers (e.g., chromium, gold, palladium) in the diode thermal balance and the influence of gold contact wire and of ceramic housing of IMPATT-diode crystal may be neglected. Also, the heat exchange between diode elements and the atmosphere may be neglected. These simplifications do not seriously affect the accuracy of the model.

The internal heat source is defined for all points within the model volume as follows:

$$\overline{Q}(z,t',T) = \frac{1}{2p}\int_0^{2p} J(j,t',T)E(x,j,t',T)\ dj \qquad (4)$$

where $j = wt$; $J(j,t',T)$ is the instantaneous IMPATT diode structure current density value; $E(z,j,t',T)$ is the electric field intensity in the point x at the time t';

This model is essentially different from the one described in [9] because here the heat source is described as the function of the electric field intensity inside the diode structure. This improvement is especially important for increasing the accuracy of the temperature distribution calculation of the active layer of the IMPATT diode.

Numerical solution of equation (3) is performed by the finite difference method. Equation (3) is solved by the alternating direction iteration method for each coordinate direction.

For this equation the alternating direction implicit method can be expressed in compact form as:

$$\frac{T_{i\ j}^{s+\frac{1}{2}} - T_{i\ j}^{s}}{t} = \frac{k}{r\ C}\left(\Lambda_1 T_{ij}^{s+\frac{1}{2}} + \Lambda_2 T_{ij}^{s}\right) + \frac{1}{r\ C} Q_j^{s}$$

$$\frac{T_{i\ j}^{s+1} - T_{i\ j}^{s+\frac{1}{2}}}{t} = \frac{k}{r\ C}\left(\Lambda_1 T_{ij}^{s+\frac{1}{2}} + \Lambda_2 T_{ij}^{s+1}\right) + \frac{1}{r\ C} Q_j^{s+\frac{1}{2}} \qquad (5)$$

$i = 1,2, \ldots I_2 - 1$; $j = 1,2,\ldots J-1$; $s = 0,1,2,\ldots\infty$;

where i, j are space coordinate numbers, s is the time coordinate number, t is the time step; I_2 is the number of x direction space coordinate nodes; J is the number of R direction space coordinate nodes. Λ_1 is the partial numerical Laplace operator on the direction r, Λ_2 is the partial numerical Laplace operator on the direction x. Two these operators are defined on the ordinary five points numerical pattern.

The temperature distribution on the first time-half-step for the nodes of numerical net is performed under the consideration that heat exchange takes place only along x coordinate. On the second time-half-step, temperature distribution is determined on the assumption that heat moves only along R coordinate.

Numerical scheme (5) has the second approximation order only. In this case it is necessary to develop the numerical net with a large number of sells for the obtaining sufficiently accuracy. That is the reason why the total computer time that is necessary for the solving of optimization problem is too large.

In this work it is proposed the other type of the thermal equation numerical approximation scheme for the accelerates of the thermal equation solving and for reducing the computer analysis time. The total analytic Laplace operator ΔT can be approximated with the numerical Laplace operator $\Lambda' T_{ij}$ as:

$$\Lambda' T_{ij} \equiv \left(\Lambda_1 + \Lambda_2 + \frac{h_1^2 + h_2^2}{12} \Lambda_1 \Lambda_2 \right) T_{ij} \qquad (6)$$

In that case we can approximate the right part of the equation (3) by the next numerical formula:

$$\frac{k}{r\ C} \Lambda' T_{ij} + \frac{1}{r\ C} \left(E + \frac{h_2^2}{12} \Lambda_2 \right) Q_j \qquad (7)$$

where E is the identity operator.

The operator Λ' is defined on the nine points numerical pattern. The approximation (6), (7) is more complicated but it has the forth approximation order. In that case we can use the numerical net that is more thin significantly for the obtaining accuracy that is equal to the scheme (5) described above. For the solution of the equation (3) by approximation (6)-(7) we used one modification of the Peaceman-Rachford numerical scheme that had been developed in the work [10]:

$$\left(E - k \cdot b \cdot \left(t - c_1\right) \Lambda_1\right) T^{s+\frac{1}{2}} = \left(E + k \cdot b \cdot \left(t + c_2\right) \Lambda_2\right) T^{s} + t \cdot b \cdot \left(E + c_2 \Lambda_2\right) Q^{s}$$

$$\left(E - k \cdot b \cdot \left(t - c_2\right) \Lambda_2\right) T^{s+1} = \left(E + k \cdot b \cdot \left(t + c_1\right) \Lambda_1\right) T^{s+\frac{1}{2}} + t \cdot b \cdot \left(E + c_2 \Lambda_2\right) Q^{s+\frac{1}{2}} \qquad (8)$$

where $b = \frac{1}{r\ C}$; $c_{1,2} = \frac{h_{1,2}^2}{12}$.

The system (8) we solve by the tridiagonal algorithm for the radial and longitudinal directions. This numerical scheme gives significant gain of computer time in comparison with the scheme (5).

The total complex nonlinear model serves as a basis for exact and complete analysis of IMPATT diodes with different doping profiles and for different operation modes.

3 Results

The model described here has been utilized for the investigation of temperature distribution in pulsed mode IMPATT diode having different doping profiles. Also, the diode admittance characteristics have been analyzed. This analysis has been performed for two types of diode structures: for the diode having a traditional even doping profile, and for the diode having the new special complex doping profile named the quasi-Read type structure.

Both of these structures are made of silicon. The first structure has the doping value $N_0 = 1.65 \cdot 10^{17}\ cm^{-3}$ for active layer. The n region length is 0.4 mm; the p region length is 0.36 mm. The second structure has two levels of active layer doping profile: $N_{min} = 1.2 \cdot 10^{17}\ cm^{-3}$; $N_{max} = 2.0 \cdot 10^{17}\ cm^{-3}$ and the n, $n+$, p, $p+$ region's lengths are 0.20 mm, 0.18 mm, 0.18 mm, 0.16 mm.

The diode numerical simulation has been performed for the following operational parameters: electrical current pulse has a square form, pulse duration t =100 nsec, period T=10 m sec. The calculated temperature distribution along the diode active layer obtained for pulse current density of 100 KA / cm^2 is shown on a Fig. 3 by the solid line for an IMPATT-diode having an even doping profile. The results obtained for the quasi-Read-type structure are also presented in Fig.3 by the dashed line.

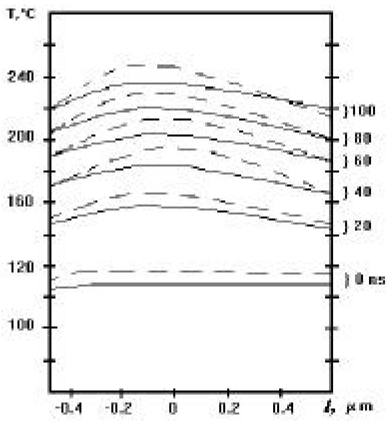

Fig. 3 The temperature distribution.

The data obtained for the diode having complex doping profile demonstrate that the inner part of this diode is hotter than that of the even doping profile diodes. This occurs because in the complex profile diode electric field intensity maximum is located further from the diode contacts than in the even doping profile diode. This means that the heat source also lies further from the contacts. Therefore, in the complex-doping-profile structure thermal flow dissipates slower than in the first structure. This also explains the existence of a larger temperature gradient along the active layer in the complex doping profile diode.

Data on the diode's active layer temperature, obtained for all time step from 0 to 100 nsec has been used for the calculation of the diode's dynamic admittance characteristics employing the nonlinear electrical model. Several examples of the calculated admittance characteristics are shown in Fig. 4.

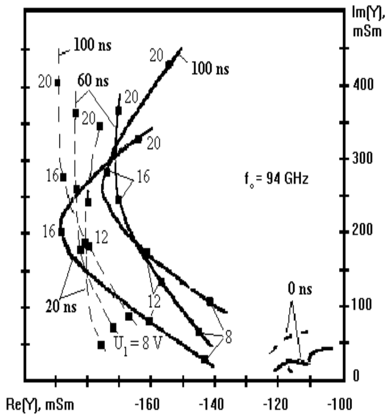

Fig. 4 Admittance frequency characteristics.

These data were obtained for the same two types of IMPATT diode doping profiles (solid lines for the even doping profile structure and dashed lines for the quasi-Read structure), and for the same operational modes as described previously. These diagrams provide complete information on diode's admittance variation with time, during the feed pulse. During the first 15 nsec the diode admittance varies very significantly. This variation is due to the strong temperature dependence of the physical parameters of silicon, in the temperature range of 100 - 170 °C. For this initial period of the feed pulse, it is possible to obtain some acceptable frequency stability only by utilizing a special external passive circuit, or by the synchronization of the signal.

During the period from 20 to 100 nsec, the imaginary part of diode admittance Im(Y) is changing more rapidly than the real part Re(Y). Relative variations of Im(Y) are around 50% of its average value. However, variations of Re(Y) are only within 5% of the average value. This demonstrates that the main cause of the generator instability is the violation of reactive energy balance during the feed pulse.

Comparison of the admittance characteristics for the two types of IMPATT diodes leads to some important conclusions. The data on the diode's admittance characteristics presented in the Fig. 4 shows that the variations of admittance value during the pulse are much less for the second structure, (dash lines) than for the first (solid lines). This can be observed in Fig. 4, where the admittance curves for the quasi-Read structure lie closer to each other, than the curves displaying the traditional even-profile diode. Therefore, the use of the complex structure, secures better frequency and amplitude stability of the generated electromagnetic oscillations. This is the principal and very important advantage of the new complex structure.

4 Conclusion

The complex numerical model of the IMPATT diode that is presented in this work takes into account the temperature distribution in the semiconductor structure and the dependence of all principal physical parameters of the semiconductor structure on temperature and the electrical field. Simultaneous use of the proposed thermal and local-field electro-dynamic models for pulsed mode IMPATT-diode analysis increases the accuracy of the diode characteristics calculation.

Comparative analysis of IMPATT diode thermal and electro-dynamic properties performed for two types different doping profiles shows that diodes with complex quasi-Read doping profile have better perspectives for use in the pulsed feed current modulation mode. This special semiconductor structure has better phase correlation between current and voltage. Therefore, complex-doping-profile diodes have improved frequency stability in pulsed-mode operation compared to the traditional IMPATT diodes having an even doping profile.

The method presented here can be applied for practical design of pulsed-mode millimetric IMPATT diodes. It can also be utilized for diode's thermal regime estimation and for the selection of feed current-pulse shape and amplitude.

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