Design Considerations for Heavily-Doped Cryogenic Schottky Diode Varactor Multipliers

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Abstract.

Diode modeling for Schottky varactor frequency multipliers above 500 GHz is presented with special emphasis placed on simple models and fitted equations for rapid circuit design. Temperature- and doping-dependent mobility, resistivity and avalanche current multiplication and breakdown are presented. Next is a discussion of static junction current, including the effects of tunneling as well as thermionic emission. These results have been compared to detailed measurements made down to 80 K on diodes fabricated at JPL, followed by a discussion of the effect on multiplier efficiency. Finally, a simple model of current saturation in the undepleted active layer suitable for inclusion in harmonic balance simulators is derived.

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I Introduction.

As diode multipliers are applied to higher frequencies (here used to mean above 500 GHz) the frequency dependent effects that can often be neglected at lower frequencies become more important. These include current saturation, carrier inertia, and capacitance of the undepleted epitaxial region [1,2]. More accurate multiplier performance predictions benefit from including these effects in the models used. Furthermore, current and future space missions are being designed to operate the LO multiplier chains at lower temperatures, near 20 K for instance [3]. Again, for accurate modeling temperature effects must be considered. These include the effects on mobility, breakdown voltage, static I/V current and current saturation. To aid in the rapid design of multipliers at many different power levels and frequency ranges, it is desirable to have models which are easy to implement using simple equations, with a minimum of arduous calculation, maximizing the speed of analysis. Thus, the more advanced models should still be fairly simple, suggesting the use of fitted equations.

As an illustration, Figure 1a shows a widely used diode model, which does a good job at lower frequencies, and can even work higher if well-calibrated. Figure 1b indicates the more sophisticated model discussed in this paper. The elements of the model will be investigated in the following sections. In section II the temperature-dependent material properties are discussed: mobility, resistivity, avalanche current multiplication and breakdown voltage. Section III is an analysis of the static junction current including the effects of tunneling, and its effect on multiplier efficiency. In section IV a simple model for analysis of current saturation in the undepleted epi region is introduced. The conclusions are presented in Section V.
II Diode Properties.

A. Mobility.

One of the primary loss mechanisms in the Schottky diode multiplier is signal absorption in the parasitic series resistance, depicted as $R_s$ in Figure 1a and $R_r$, $R_m$, and $R_{\infty}$ in Figure 1b. The value of these resistances is proportional to the resistivities in the active epitaxial layer, the highly-doped sub-layer, and ohmic contacts respectively. Resistivity depends on the low field mobility, which can either be calculated by Monte Carlo methods [4-6] or measured [7, 8]. To facilitate calculation of the mobility for rapid design, a fitted algebraic equation is desired, including the effects of temperature and donor concentration. The author is not aware of a good fit, so the following expressions are suggested:

$$
\mu = \left( \frac{1}{\mu_0} + \frac{1}{\mu_f} \right)^{-1}
$$

$$
\mu_0 = \frac{2296 \text{ cm}^2/\text{Vs}}{\left[ \exp\left(\frac{490}{T}\right) - 0.42 \right]^{-1} + \left(\frac{T}{3410}\right)^3}
$$

$$
\mu_f = \left[ \frac{1}{\left(\frac{184}{T}\right)^3 + 1} \right] \left[ \frac{2.34 \times 10^3 \left(20/T\right)^4 \left(\frac{n_0}{10^{14}} \left(1 + \theta \right) \left(1 - \theta \right)^{0.86 - T/900} + 10^4 \theta^{0.68 - 0.27} \right)}{T/163 + 0.8} \right] \text{ cm/Vs}
$$

where $T$ is the temperature in Kelvins, $n_0$ is the carrier concentration in cm$^{-3}$, and $\theta$ is the compensation ratio, defined [5] as the ratio of ionized acceptor to ionized donor concentrations. Since the normal donors in GaAs, such as Si, are shallow (~6 meV), as the carrier concentration increases the donor levels merge with the conduction band [9]. This occurs at a donor concentration of around $10^{16}$ cm$^{-3}$, and above that all donors are considered ionized except at extremely low temperatures, 10 K or so. Since the range of temperatures considered here is above 50 K and donor concentrations are above $10^{17}$ cm$^{-3}$, the carrier concentration is assumed equal to effective donor concentration, $N_D - N_A$, where $N_D$ and $N_A$ are the donor and acceptor concentrations.

The resistivity $\rho$ is given by the usual formula:

$$
1/\rho = q\mu n_a
$$

Figure 2 shows a plot of resistivity versus carrier concentration. Our room temperature and 100K calculations based on the formula above are compared to the room temperature plot in [10].

B. Avalanche current multiplication and breakdown.

Avalanche current multiplication caused by impact ionization is important in the reverse bias regime, especially for the highly doped diodes being used. This is the mechanism for junction breakdown, assuming the epi region is thicker than the depletion width when it occurs. Avalanche multiplication increases the current injected from one side of the depletion region by a factor $M$. Since impact ionization occurs at high fields, around $5 \times 10^5$ to $10^6$ V/cm, it occurs first under the anode at high reverse bias, that is, the current being multiplied is comprised of electrons penetrating the barrier from the anode contact. Under these circumstances, $M$ is given by [11]:

$$
1 - \frac{1}{M} = \int_0^W \alpha_s \exp \left[ - \int_0^{x'} (\alpha_s - \beta_h) dx' \right] dx
$$

where $\alpha_s$ is the field-dependent electron ionization coefficient, $\beta_h$ is the corresponding hole ionization coefficient, and $W$ is the depletion width at the given voltage. To determine the breakdown voltage, $M$ is taken to be infinite,
and the right side of (3) is solved iteratively to determine the applied voltage and corresponding field distribution and depletion width that make it unity.

Many researchers over the years have attempted to determine the ionization coefficients of GaAs [12-16]. For this work the measurements reported by Bulman et al. [14, 15] were used. Baraff [17] made calculations parameterizing the ionization coefficients at low temperature in terms of the optical phonon energy $E_r$, the mean free path between phonon scattering events $\lambda$, and the average ionization energy, $E_i$. These have been extended to all temperatures [18] using the assumption that $E_i$ varies with temperature as the band gap energy and that $E_r$ and $\lambda$ vary as:

$$\frac{E_r}{E_{r0}} = \frac{\lambda}{\lambda_0} = \tanh\left(\frac{E_{r0}}{2kT}\right)$$

where the zero subscripts refer to zero Kelvin values. The 0 K phonon energy is known to be 0.036 eV, so only values for $E_i$ and $\lambda_0$ must be determined. The calculations in [17] have been fitted by Okuto and Crowell [18] to a simple formula. For our study the expression in [18] has been modified to fit Baraff’s data more closely, which seems to model the measurements better. The modified equation is:

$$\alpha \lambda = f \left[\frac{b}{x} \exp[a - \sqrt{a^2 - x^2}]\right]$$

Here $\alpha$ is either $\alpha_e$ or $\beta_e$ as appropriate, $f$ is a simple factor which accounts both for variations in measurements and for the unknown ratio of impact ionization cross-section to phonon emission cross-section [17]. The expressions for $a$, $b$, and $x$ are:

$$a = 0.116 \left(\frac{E_i}{E_{r}}\right)^{1.266} \quad b = 6.83 \left(\frac{E_r}{E_{i}}\right) + 0.113 \quad x = \frac{E_{r}}{qE_{\lambda}}$$

with $E$ being the magnitude of the electric field. For this work values for the parameters that fit well to Bulman’s data are: $E_i = 2$ eV and $f = 0.44$ for both electron and hole ionization coefficients, and $\lambda_0 = 78.6$ Å for $\alpha_e$ and 71.1 Å for $\beta_e$. As pointed out in [15, 19, 20] the ionization coefficients also depend on location. The effect of this was checked using the model of [15, 20], and it was found that for doping up to about $5 \times 10^{17}$ the difference in breakdown voltage with and without this correction is only a few tens of millivolts.

Figure 3 shows the breakdown voltage calculated using the ionization coefficients from equation (5) in equation (6) at 300 K, compared to a plot from [21] based on Pearsall's coefficients [13]. Also shown as scattered points are measurements used to derive the coefficients in [14, 15] as well as others as reported in [22, 23]. The fit is better to those using Bulman’s data at lower doping, although the difference between the two calculations is very small for the more highly doped diodes. Also shown is a curve indicating the breakdown voltage at 100 K calculated as above. Again, the temperature dependence is small at the higher dopings.

III Junction Current.

Quantum mechanical electron tunneling through the Schottky barrier is the dominant static current mechanism in low temperature and in highly doped diodes. This is because at high doping levels the depletion width is narrow, giving the large number of electrons below the top of the barrier a substantial probability of tunneling through. At lower donor concentrations the depletion width is great enough that the dominant current mechanism is thermionic emission over the barrier. Several approximate tunneling current calculations were developed by Padovani and Stratton and others [24-27], but due to the approximations in calculating the tunneling coefficient the results are not valid over all current regimes. Recently the transfer matrix technique has been used [28, 29] to calculate the tunneling currents [30, 31]. This is a type of mode matching
algorithm wherein the barrier is divided up into a series of slices, each having a constant or linear potential profile. After the transmission coefficient, \( T(E_n) \) is calculated for each value of the normal component of electron energy, \( E_n \), the current density is calculated according to [32, equation (13)]. The transmission coefficient depends on the potential profile, including the barrier height, \( \phi_b \), which is given for an anode at \( x = 0 \) by:

\[
\psi = \phi_b - qE_{\text{max}} \left( 1 - \frac{x}{W} \right) - \frac{q^2}{16\pi\varepsilon_0\varepsilon_r x}
\]

with \( \varepsilon_r \varepsilon_0 \) the semiconductor dielectric constant. The electric field under the anode is given as:

\[
E_{\text{max}} = \sqrt{2q(N_D - N_A)\phi_b - V - V_n} / \varepsilon_r \varepsilon_0
\]

where \( V_n \) is the difference in potential between the Fermi level and the bottom of the conduction band in the semiconductor bulk. The barrier height itself commonly appears to have a dependence on the applied voltage [10, 33, 34]. For this work, the barrier height is characterized by an asymptotic "flat-band" height, \( \Phi_{FB} \), which is the barrier height at zero electric field, when the conduction bands would be flat. Additionally, the barrier height is assumed to have a linear dependence on \( E_{\text{max}} \):

\[
\phi_b = \Phi_{FB} - \alpha E_{\text{max}}
\]

Since \( E_{\text{max}} \) and \( \phi_b \), are mutually dependent, they must be solved for together as discussed in [33].

![Block Diagram and photo of cryostat set up and wire-bonded diode.](image)

To check the validity and determine the effect of the tunneling current on multiplier performance, several diodes fabricated at JPL have been measured over a wide temperature range in a specially designed cryostat [35]. The cryostat, shown in Figure 4, consists of a vacuum chamber enclosing the device under test (DUT) cooled by a two-stage closed-cycle Helium refrigerator. The temperature of the DUT is adjustable to within \( \pm 1 \) K in the 35-325 K range using a temperature controller with two temperature sensors, a 25 W heater and a bracket that mechanically connects the DUT to the 15 K second stage cold plate of the refrigerator.

The HP 4155B Semiconductor Parameter Analyzer is connected to the DUT with four cables for a four-probe measurement, compensating for the series resistance of the lines (Figure 2). Shielded cables connect the analyzer to SMA adaptors at the vacuum flange of the cryostat where the signals are fed through into the chamber. Inside the cryostat short sections of flexible cable connect the feed-through to the ceramic test socket which is
thermally bonded through a copper block to the temperature-stabilized cold plate. The diode is epoxied to the test socket and connected with four 25 μm bond wires to the carrier as also shown in Figure 4.

A diode fabricated a JPL on material doped to 3×10⁷ with an anode size of 1.5×10.5 μm² was measured from 100 to 300 K. The magnitude of the measured and calculated currents are compared in Figure 5. The current calculations included tunneling and avalanche multiplication as described earlier. Values of \( \Phi_{FB} = 0.92 \) eV and \( \alpha = 30 \) Å in equation (11) were used to fit the measurements. The fit is pretty good, but it is desirable to have independent justification for these values. The flat-band barrier height is dependent on the metal/semiconductor system in the contact. Using forward bias measurements of the reverse saturation current and ideality factor, the flat-band barrier height and effective barrier height, \( \Phi_{eff} \) can be determined as discussed in [36-39] based on the fact that as the applied voltage approaches the built-in voltage (flat-band), all current mechanisms except thermionic approach zero. This includes tunneling (because the bulk of electrons are near the barrier top in energy) and any models described by a linear field dependence (since the field approaches zero). This type of analysis was also performed on the above diode, with the results shown in Figure 6a. Since the JPL anodes are fabricated from Ti/Pt/Au, the flat-band barrier height should be compared to those metals. In [38] the reported heights are around 0.83 eV for Ti, 0.92 eV for Au and 0.99 eV for Pt. The measured values fit a line \( \Phi_{FB} = 0.95 - 0.0003T \) eV, \( T \) being the temperature in Kelvin. It is possible that some intermixing may be taking place between the Ti and the Pt, but this cannot be said for certain. As to the \( \alpha = 30 \) Å factor, many theories have been proposed explaining non-zero \( \alpha \) as due to the imperfect nature of the metal-semiconductor interface [33, 34, 40-44]. Again, there is not enough data to pin this down.

Figure 5. Tunneling/avalanche current calculations compared with measurement. The solid lines are measured currents, broken lines are calculated.
with a model wherein the shunt conduction is a surface "hopping" phenomenon, where the carriers do freeze out as the temperature drops. Generation-recombination current was considered, but it is proportional to the product of depletion width $W$ and intrinsic carrier concentration $n_i$. For GaAs in general $n_i$ is very low and for highly doped diodes $W$ is small, so this current mechanism is insignificant in this case.

To evaluate the effect of these departures from thermionic behavior on multiplier efficiency, a simple model consisting of two diodes back-to-back was incorporated into a commercial harmonic balance simulator. A schematic is shown in Figure 7. One diode models the forward current, the other the reverse. The fit of the modeled current magnitude to the measurements is also shown in Figure 7. The fit is good for the forward bias, and not so good for reverse. However, the fit at the higher reverse currents is good, and the lower currents should have little effect on the performance of the multiplier.

Performance calculations of a 200 GHz multiplier with and without the reverse tunneling component are shown in Figure 8. As can be seen, at room temperature there is a significant reduction in efficiency when tunneling current is considered, but at 100 K there is no substantial difference. There is also no observed difference when the same calculation is performed at 800 GHz. These can be explained by noting that all Schottky multipliers suffer from two loss mechanisms: series resistance loss, which dominates, and conduction current loss. As the temperature is lowered, the conduction current drops (at a given voltage) so the conduction current contribution to the loss is greatly reduced. Hence, little difference in efficiency occurs with or without tunneling at low temperatures. At 800 GHz the efficiency is low and also greatly dominated by the series resistance loss, so the exact conduction current mechanism has little effect on efficiency.

IV Current Saturation.

As the electric field in a GaAs sample is increased, the velocity and hence the current reaches a peak, then begins to decline due to electrons gaining enough energy from the field to scatter into the upper, low-mobility valleys. This acts as a current limit in the undepleted epitaxial region of the diode. Current saturation reduces the efficiency of the diode as a multiplier because it decreases the ability of the charge at the edge of the depletion region to move around at the signal frequency and modulate the capacitance, generating the varactor non-linearity. There are also time constants associated with the transfer, and at the high frequencies being considered here they should be taken into account.

There are several equations used to describe the static current saturation profile. The simplest and oldest is the Kramer and Mircea formula [47]:

$$u(F) = \frac{\mu_s F + u_s (F / F_u)^4}{1 + (F / F_u)^4}$$

where $u$ is the velocity, $F$ the magnitude of the electric field, $u_s$ the ultimate saturation velocity at about 20 kV/cm, and $F_u$ is a characteristic field which determines where the peak velocity occurs. Usually current saturation, including transient effects have been modeled using Monte Carlo simulations (see, for example [45, 46]). Since
Monte Carlo calculations take large amounts of computer time, it is desirable to incorporate these effects into a harmonic balance (HB) circuit simulator using a simple model which can be integrated using the Runge-Kutta type integrators normally used in HB simulators. We propose to use a time constant based formulation somewhat similar to that introduced in [48]. The epi current is divided between two resistances representing the dominant two conduction band valleys in which electrons travel, as illustrated in Figure 9. Defining $\mu_0$ as the lower valley mobility, (about 4000 cm$^2$/Vs or higher at reduced temperatures), and $\mu_i$ is the upper valley mobility (about 400 cm$^2$/Vs) and $n_0$ and $n_i$ as the corresponding valley populations, the velocity in equation (12) can be written:

$$u(F) = \left( \frac{\mu_0 n_0}{n} + \frac{\mu_i n_i}{n} \right) F$$

with $n$ the total electron concentration in the undepleted epi. Then, several coupled differential equations are used to represent the time-dependent behavior of the velocity. The upper valley population is described by:

$$\frac{dn_i}{dt} = \frac{n_{is}(V) - n_i(t)}{\tau}$$

where $n_{is}(V)$ represents the static population of the upper valley, derived by combining equations (12) and (13) and noting that the total electron concentration is the sum of the populations of the two valleys, i.e. $n = n_0 + n_i$. The time constant, $\tau$ is dependent on the voltage across the epi, $V_{sat}$.

The current through the inductor representing carrier inertia has the usual equation:

$$\frac{di}{dt} = \frac{V_{sat}(t) - V(t)}{L_i}$$

where $L_i$ is the carrier inertia inductance, equal to:

$$L_i = \frac{m^* w}{q^2 nA}$$

with $m^*$ the effective mass, $w$ the thickness of the undepleted epi, and $A$ the area of the diode. The total current through the inductance is simply:

$$i = nuA.$$
It was found that values for \( r \) ranging linearly from 0.2 ps at the 20 kV/cm to 3 ps at 1 kV/cm gave a good fit. As a further test, the same model is compared in Figure 11 with a sinusoidal 60 GHz excitation of 10 kV/cm amplitude. Again, the match is good. Also plotted is the current through a resistance having a mobility one-third that of GaAs (hence three times the resistance), which gives an estimate of the magnitude in performance reduction.

Currently, it appears that the above model, simple as it is, is impossible to incorporate into commercial HB simulators. Work is continuing in this direction, and a version of the Siegel/Kerr reflection algorithm [49] is in progress so this model can be used to actually design multipliers.

V Conclusions.

Several suggestions have been made for improving the modeling of Schottky diodes for high doping and frequency, and low temperatures. The effects examined have been low-field mobility, breakdown, conduction current, barrier height and current saturation. Most of the effects serve to merely reduce the achievable efficiency, but not change the designs themselves very much, specifically the matching impedances. This is because the most important design parameter is the reactance tuning, dominated by the diode capacitance, which has been accurately modeled previously. However, the current saturation serves to greatly increase the effective series resistance, which is the dominant loss mechanism. It is possible to estimate the magnitude of the effect by using a series resistance much larger than the measured DC values in the performance estimates [50]. However, by calculating the behavior of current saturation with variations in doping and temperature, it should soon be possible to improve the optimization of the doping and anode sizes of high frequency multiplier diodes.

References

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