

Model of Schottky junction admittance taking into account incomplete impurity ionization and large-signal effects

Andrei V. Los* and Michael S. Mazzola

Mississippi State University, Department of Electrical and Computer Engineering, Box 9571, Mississippi State, Mississippi 39762

(Received 17 October 2001; published 5 April 2002)

A general model for the Schottky junction reverse bias admittance is created. The model takes into account incomplete impurity ionization and does not rely on the small-signal approximation, so that impurity rate equations are not linearized. The model is valid at arbitrary temperatures for an arbitrary periodic bias amplitude and harmonic content as long as the free-carrier relaxation time is much shorter than the bias period. Impurity ionization is treated in the framework of the Shockley-Read-Hall statistics; free-carrier distribution is assumed to be an equilibrium one. The model allows calculation of the junction potential distribution and thus the junction transfer function and admittance. Junction admittance is calculated for different ac bias amplitudes and the results are compared with the data obtained from the small-signal model. It is shown that the model fits experimental junction admittance more accurately than the small-signal model when the ac component of the potential is large with respect to the thermal potential $k_B T/q$.

DOI: 10.1103/PhysRevB.65.165319

PACS number(s): 73.30.+y, 73.40.Ns

I. INTRODUCTION AND BACKGROUND

Semiconductor junction admittance is one of the most important junction characteristics. Accurate description of this quantity is important for semiconductor device characterization and simulation. In most cases admittance of an ideal junction is considered to have only the imaginary part, the capacitance; the real part, the conductance, results from the junction nonideality, i.e., leakage. The junction capacitance is usually described using Schottky's formula^{1,2}

$$C = \sqrt{\frac{q\epsilon N_d}{2(\varphi_B - V_A)}},$$

where N_d is the semiconductor doping impurity concentration, ϵ is its permittivity, φ_B is the junction built-in potential, V_A is the applied bias voltage, and q is the electronic charge. This formula, although accurate enough in many cases, is based on several assumptions which may not be satisfied in a number of important applications. First, the depletion approximation is assumed to be valid. In reality, particular potential and charge distributions, which are functions of several factors such as doping occupation and applied bias, affect the junction admittance. Second, it is assumed that impurities are completely ionized throughout the semiconductor. This is typically true for doping impurities in traditional semiconductors such as Si or GaAs at room temperature. However, the degree of ionization of common dopants may be far from unity in such wide band-gap semiconductors as SiC or GaN even at room temperature. Some degree of carrier freeze out may also be present in a semiconductor containing deep traps or at lower temperatures.

If an ac bias, such as an impedance meter measurement signal, is applied to a junction and incomplete impurity ionization is present, the ac signal may lead to periodic impurity ionization/neutralization in a vicinity of the point of intersection of the impurity level with the corresponding quasi-Fermi level. This charge change results in an additional component in the junction admittance, which is not taken into account in

Schottky's formula (because it takes into account only the free carrier sweep out at the space-charge region boundary). Impurity ionization processes are not instantaneous and, if the ionization time constant is comparable to or larger than the ac bias period, these processes will lag the bias changes. In this case the junction admittance will be frequency dependent and will contain a conductive component. At very high frequencies or at low temperatures when the free-carrier relaxation time becomes comparable with the ac signal period, the lag in the free-carrier response needs to be accounted for as well.

The effects of incomplete impurity ionization on the junction admittance have been confirmed experimentally by a number of authors.³⁻⁸ First theoretical treatment of the junction admittance in the presence of an incompletely ionized impurity was performed by Vul, who calculated the capacitance of a *pn* junction at an arbitrary temperature (and, therefore, impurity fractional ionization).⁹ The author did not use impurity ionization statistics; therefore, the obtained capacitance value is that for the low-frequency limit. Also, the author used the depletion approximation. The expression obtained for the capacitance coincides with Schottky's formula, which is a natural result since under the depletion approximation the impurities are assumed to be completely ionized in the entire depletion region by the electric field. Roberts and Crowell¹⁰ have given an exact expression for the low-frequency Schottky junction capacitance. This expression is valid for any number of impurities with arbitrary ionization energies at any temperature, as long as the impurity ionization processes respond to bias changes instantaneously, and properly takes into account the junction potential distribution, i.e., without assuming the depletion approximation or its variants.

To correctly describe the situation when the impurity ionization time constant is comparable with the ac bias period, and the impurity ionization processes occur out of phase with the bias, an analysis which would include a description of the probabilistic impurity ionization processes is needed. Such an analysis was first done by Sah and Reddi⁴ for the capaci-

tance of a pn junction containing a single deep level. The authors used the truncated space-charge approximation and Shockley-Read-Hall statistics^{11,12} for trap centers to obtain expressions for the junction capacitance as a function of applied dc bias in low- and high-frequency limits. In the truncated space-charge approximation Poisson's equation is simplified by introducing a piecewise-constant space-charge distribution under the assumption that deep impurities change their charge state from zero to unity due to a bias change only in the point where the impurity energy level intersects the corresponding quasi-Fermi level. This approximation therefore does not allow correct calculation of the magnitude of the space-charge region charge change due to the impurity ionization and also implies a single impurity time constant instead of a time constant distribution in the region where impurity charging-discharging takes place, leading to an inaccurate calculation of the frequency dependence of the junction admittance.

Another approximation Sah and Reddi made is that the ac potential does not change the free carrier and the ionized impurity concentrations significantly, so that the changes in these quantities can be treated as perturbations, and mean values of these quantities are approximately equal to their static (when only the dc bias is applied) steady state values. This approximation is equivalent to the assumption that the ac potential is small with respect to $k_B T/q$ in the regions where potential changes can lead to changes of other junction parameters, i.e., the small-signal approximation. The small-signal approximation allows linearization of impurity rate equations and transformation of the Poisson equation to use the static potential as the independent variable, so that calculation of the junction admittance can be done without finding an explicit solution for the potential.^{6,10} The approximation, however, is valid only in a limited range of ac voltages and temperatures. For example, a standard ac measurement signal used in impedance meters is 30 mV rms. The amplitude of this signal is about 42 mV, which is larger than $k_B T/q$ at room temperature. Impurity charging-discharging takes place in the depletion region tail, where the value of the ac potential is smaller, so one can hope that in this region the small-signal approximation is valid. However, for larger ac bias amplitudes and at lower temperatures a model which does not rely on the small-signal assumption is needed.

Several authors obtained expressions for the junction admittance without using truncated space-charge or single time constant approximations. Perel and Efros¹³ obtained low- and high-frequency expressions for the pn junction capacitance by artificially introducing an impurity time constant distribution as a function of the ratio of shallow and deep impurity concentrations. Forbes and Sah¹⁴ used the equivalent circuit approach to model pn junction small-signal capacitance and conductance in the presence of a single deep trap. The model takes into account the true impurity time constant distribution but is valid only at zero bias and cannot be easily extended to other bias conditions. Oldham and Naik⁷ obtained expressions for the capacitance and conductance of a pn junction with a trap as a function of frequency. They modified the truncated space-charge approximation slightly and used finite-thickness charge sheets to model the

regions where impurity ionization takes place. Beguwala and Crowell¹⁵ calculated the small-signal admittance of a junction device at an arbitrary temperature and frequency in the presence of multiple deep traps with arbitrary time constant distributions and synthesized the junction equivalent circuit for this case. This treatment requires numerical integration. The conductive component of the admittance is expressed as the imaginary part of the capacitance. A very general treatment of the Schottky junction admittance has been presented by Losee.⁶ The author extends the approach of Roberts and Crowell¹⁰ to any ac bias frequency. The author's model of the Schottky junction admittance is valid for any number of impurity species and any ac bias frequency, and takes into account (implicitly) a particular potential and impurity time constant distributions in the junction space-charge region. The model requires numerical integration and is again valid only in the small-signal case. This model is the most general small-signal model and will be compared with the general large-signal model that we develop in this paper.

An attempt to overcome the limitations of the small-signal approximation and calculate the reverse bias junction admittance for an arbitrary ac bias amplitude was made by Frandon and Hoffmann in a series of papers.¹⁶⁻¹⁸ The authors took a general expression for the junction capacitance bias dependence $C = C_0 \varphi_B^\alpha (\varphi_B - V_A)^{-\alpha}$ and used the specific sinusoidal excitation $V_A = V_e \cos \omega t$ with an arbitrary amplitude V_e to calculate the junction capacitance change from its small-signal value as a function of the ac to dc bias ratio. This approach, however, has a limited applicability and accuracy, since it fails to take into account particular potential or charge distribution changes caused by the ac bias being large or the impurity ionization effects.

In this paper we develop a very general reverse bias Schottky junction admittance model, which does not rely on either the small-signal or the truncated space-charge approximation. It is valid at arbitrary temperatures for an arbitrary periodic bias amplitude and harmonic content and arbitrary impurity energy-level distributions (changes in the free-carrier relaxation time are not considered). In the next section, we present theoretical development of the model. In Sec. III, we perform admittance calculations using the model and the general small-signal model. We show the influence of the applied ac bias amplitude on the junction admittance. In Sec. IV, we present experimental data for the junction admittance in a temperature range where the small-signal condition is not satisfied and compare least-squares fits of the general and small-signal models to the data. The results of this paper are summarized in Sec. V.

II. THEORY

In the development of the model we will make several assumptions. First, it is assumed that the junction is in the dark, the leakage currents are negligible, and the dielectric relaxation time is much shorter than the maximum ac bias period under consideration. The latter condition may not be satisfied at very low temperatures when the carriers are freezing into the shallowest impurity. We assume that this occurs at temperatures lower than the temperature at which

the impurity ionization processes affect the junction admittance. These assumptions allow us to treat the free-carrier distribution as in equilibrium, so that the carrier density can be calculated simply from the Fermi-Dirac or Boltzmann statistics, without the need to take into account the free-carrier density time dependence or the Fermi level changes caused by excessive carriers.

Next, it is assumed that Shockley-Read-Hall statistics are applicable for impurities. With this model limitations in capture or emission rates arise only from the availability of an electron to enter the impurity and the existence of an impurity state which could accept this electron. It is assumed that once the electron is captured, it can be reemitted instantly (with the corresponding probability, which is a function of temperature, local electric field, and impurity parameters). Another possible process, namely, the readjustment of the electron in the impurity after the capture act, is neglected. That is, it is assumed that the electron is captured directly into the ground state, or that its transition to the ground state is instantaneous, or that the probability of its emission from any other state in which it could be captured is the same as from the ground state.¹¹

In general, the application of an arbitrary bias to the semiconductor junction results in the excitation of an infinite number of junction current harmonics. The total current can be represented in a Fourier integral or, if the current is periodic, in a Fourier series form. The junction can then be described by its transfer function \mathbf{Y} , which relates the amplitudes of the current harmonics to the amplitudes of the applied bias harmonics and satisfies the equation $\mathbf{J}=\mathbf{Y}\mathbf{V}$, where \mathbf{J} is the current density vector and \mathbf{V} is the bias voltage vector. Both the current and voltage vectors have, in general, infinite dimension and are complex, which takes into account any existing phase shifts; the transfer function is an infinite dimension complex matrix. Since junction leakage currents are neglected, the total current at the semiconductor-metal interface contains only the displacement component, and thus the matrix elements y_{kl} of the transfer function in the case of periodic bias with m harmonics can be calculated as follows:

$$y_{kl} = \frac{-ik\omega\epsilon}{m} \left(\frac{1}{\varphi_l} \frac{d\varphi_k}{dx} \right)_{x=0},$$

where φ_k are the components of the junction potential vector (band-edge energy measured relative to its value in the bulk), and the point $x=0$ corresponds to the semiconductor-metal interface.

When the junction admittance (or impedance) is measured by an impedance bridge, a sinusoidal measurement signal of amplitude V_{ac} is applied to the junction together with a (possibly zero) static bias of amplitude V_{dc} . Usually the measurement circuit of the impedance bridge filters out all harmonics of the junction current but one, corresponding to the frequency of the measurement ac signal.¹⁹ The ratio of the amplitude of this harmonic of the current to V_{ac} is the measured junction admittance, which can be defined as

$$Y \equiv y_{11} = -i\omega\epsilon \left(\frac{1}{\varphi_1} \frac{d\varphi_1}{dx} \right)_{x=0}. \quad (1)$$

To find the junction potential one has to solve Poisson's equation

$$\frac{d^2\varphi}{dx^2} = -\frac{q}{\epsilon} \left(\sum_d N_d^+ - \sum_a N_a^- - n + p \right), \quad (2)$$

where N_d^+ is the concentration of ionized donor species, N_a^- is the concentration of ionized acceptor species, and n and p are electron and hole concentrations, respectively. Since the ac bias can have any value, all, or at least several, harmonics of the junction potential need to be taken into account. A large ac potential can significantly change the mean values of the junction parameters compared to their static values, and these changes will not be proportional to the potential; the junction static potential will not define the mean values of the junction parameters anymore, and thus cannot be used as the independent variable, so that Poisson's equation cannot be transformed correspondingly.

Since it is assumed that free carriers are in thermal equilibrium, the corresponding quasi-Fermi levels are gradient-free, and the continuity equation contains only generation and recombination terms which compensate each other. Thus, this equation does not introduce anything new into the problem and can be omitted. Neglecting multiple charging effects, impurity occupation can be calculated from a set of standard Shockley-Read-Hall equations¹¹ for each impurity species

$$\frac{\partial N_d^+}{\partial t} = e_n(N_d - N_d^+) - C_n n N_d^+ - e_p N_d^+ + C_p p(N_d - N_d^+), \quad (3a)$$

$$\frac{\partial N_a^-}{\partial t} = e_p(N_a - N_a^-) - C_p p N_a^- - e_n N_a^- + C_n n(N_a - N_a^-), \quad (3b)$$

where N_d and N_a are concentrations of electrically active donor and acceptor impurities, e_n and e_p are electron and hole emission coefficients, and C_n and C_p are their capture coefficients, which are all assumed to be independent from the particular conduction- or valence-band state which a charge carrier is emitted to or captured from. For a semiconductor with nondegenerate free electron and hole distributions, the carriers are captured from and emitted to the states near the conduction- or valence-band edge, and this condition is satisfied.

For donors in the upper half of the forbidden band and acceptors in its lower half, interaction with valence and conduction band, respectively, can often be neglected, which means that the corresponding capture and emission coefficients in Eqs. (3) can be set equal to zero. To make further derivation more concise we consider a single donor impurity to be present in the semiconductor. The results will then be generalized to any number of donors or acceptors. After these simplifications, the donor impurity rate equation becomes

$$\frac{\partial N^+}{\partial t} = e_n(N - N^+) - C_n n N^+, \quad (4)$$

where the subscript “ d ” is omitted for brevity.

By assuming continuity of the potential and its derivative, it easily follows that for an arbitrary periodic bias at a time sufficiently long after any transient processes following the bias application have passed, the junction will be in a steady state with the potential and ionized impurity and free-carrier concentrations being periodic functions, which can be represented in a Fourier series form

$$N^+ = N_0^+ \sum_{k=-\infty}^{\infty} a_k e^{ik\omega t},$$

$$n = n_0 \sum_{k=-\infty}^{\infty} b_k e^{ik\omega t},$$

$$\varphi = \beta \sum_{k=-\infty}^{\infty} c_k e^{ik\omega t},$$

where $\beta \equiv k_B T/q$, n_0 , and N_0^+ are the electron and ionized impurity concentrations in the semiconductor bulk, respectively, and Fourier coefficients b_k and c_k are given by

$$b_k = \frac{\omega}{2\pi} \int_{-\pi/\omega}^{\pi/\omega} \frac{n}{n_0} e^{-ik\omega t} dt,$$

$$c_k = \frac{\omega}{2\pi} \int_{-\pi/\omega}^{\pi/\omega} \frac{\varphi}{\beta} e^{-ik\omega t} dt.$$

Substituting Fourier expansions for n and N^+ in the rate Eq. (4), the following system of linear equations is obtained for a_k :

$$a_k(i\omega k + \tau^{-1}) + C_n n_0 \sum_{m=-\infty, m \neq k}^{\infty} a_m b_{k-m} = 0, \quad k \neq 0, \quad (5a)$$

$$a_0 \tau^{-1} + C_n n_0 \sum_{m=-\infty, m \neq 0}^{\infty} a_m b_{-m} = e_n \frac{N}{N_0^+}, \quad (5b)$$

where $\tau = (e_n + C_n n_0 b_0)^{-1}$ is defined as the impurity ionization time constant.⁶ System (5) allows the Fourier coefficients a_k of the ionized impurity concentration to be calculated if Fourier coefficients b_k of the free-carrier concentration are known.

The free-carrier concentration n should, in general, be found using Fermi-Dirac statistics, so that Fourier coefficients b_k are given by

$$b_k = \frac{\omega}{2\pi} \int_{-\pi/\omega}^{\pi/\omega} \left[\frac{1}{n_0} \int_{E_c}^{\infty} g(E) f(E - \varphi, \mu_F) dE \right] e^{-ik\omega t} dt,$$

where $g(E)$ is the conduction band density of states and $f(E, \mu_F)$ is the Fermi distribution function. The bulk values of the free-electron concentration n_0 and the Fermi level μ_F can be found from a charge neutrality equation. To make

further discussion more concise we will assume that the free-carrier distribution is not degenerate, Boltzmann statistics apply, and n is given by $n = N_C e^{(E_c - \mu_F)/k_B T} = n_0 e^{-\varphi/\beta}$. In this case expression for the Fourier coefficients b_k is simplified

$$b_k = \frac{\omega}{2\pi} \int_{-\pi/\omega}^{\pi/\omega} \exp\left(\sum_{l=-\infty}^{\infty} c_l e^{il\omega t}\right) e^{-ik\omega t} dt. \quad (6)$$

In the small-signal case $|c_{\pm 1}| \ll 1$ and $c_k = 0$ for $|k| > 1$. Then, the exponent in the integral for b_k can be represented by only the zero and first-order terms of its Taylor expansion $e^{c_0}(1 + c_{-1}e^{-i\omega t} + c_1 e^{i\omega t})$. Consequently, only b_k with $|k| \leq 1$ are nonzero and are given by: $b_0 = e^{c_0}$, $b_{\pm 1} = e^{c_0} c_{\pm 1}$. This result is expected since in the small-signal case the free-carrier concentration change is linear in the ac potential. Next, neglecting second-order terms in Eq. (5), Fourier coefficients a_k are found as follows:

$$a_0 = \frac{e_n}{\tau^{-1}} \frac{N}{N_0^+},$$

$$a_{\pm 1} = -\frac{C_n n_0}{i\omega + \tau^{-1}} a_0 b_{\pm 1},$$

$$a_k = 0, \quad |k| > 1.$$

The solution for a_1 is the same as given by Losee's small-signal model for the proportionality coefficient between the ac potential and the corresponding junction charge change.⁶ The expression for a_0 can be rewritten in the following form:

$$e_n(N - a_0 N_0^+) - C_n b_0 n_0 a_0 N_0^+ = 0.$$

Here, $b_0 n_0$ and $a_0 N_0^+$ are mean values of the free-carrier and ionized donor concentrations, and this relation expresses the fact that in the small-signal case the junction is in a quasi-equilibrium state with the capture and emission processes compensating each other. For an arbitrary amplitude ac bias, as it follows from Eq. (5), the mean value of the ionized impurity concentration a_0 depends on the junction potential harmonics of nonzero order.

Using the Fourier expansions for N^+ and n , Poisson's equation is transformed into a system of differential equations for c_k

$$\frac{d^2 c_k}{dx^2} = -\frac{q}{\varepsilon \beta} (N_0^+ a_k - n_0 b_k), \quad k = 0, 1, 2, \dots, \quad (7)$$

Each Eq. (7) is a two-point second-order boundary-value problem for c_k , which should be solved numerically (note that the Fourier coefficients with the indices having opposite signs are complex conjugate, and thus, only the coefficients with positive indices need to be calculated). For the case of a sinusoidal applied bias, the boundary conditions are

$$c_0(0) = (\varphi_B - V_{dc})/\beta, \quad c_1(0) = V_{ac}/\beta,$$

$$c_k(0) = 0, \quad k > 1,$$

$$c_k(\infty) = 0, \quad k = 0, 1, 2, \dots, \quad (8)$$

The system of Eqs. (7) allows one to calculate junction potential distribution, the junction transfer function coefficients and, as a particular case, its admittance for the case of a single donorlike impurity in a semiconductor with electrons being the majority carriers and a negligible hole concentration. This system is easily generalized to the case of a semiconductor with an arbitrary number of impurity species, provided their energy levels are situated far from the middle of the forbidden band so that interaction of the donorlike impurities with the valence band and interaction of the acceptorlike ones with the conduction band is negligible

$$\frac{d^2 c_k}{dx^2} = -\frac{q}{\epsilon\beta} \left(\sum_d N_{d0}^+ a_{dk} - \sum_a N_{a0}^- a_{ak} - n_0 b_k + \frac{p_0}{b_k} \right),$$

$$k=0,1,2,\dots, \quad (9)$$

where indices “ d ” and “ a ” denote summation over all donor and acceptor impurities, respectively. Note that, since equilibrium electron and hole concentrations are assumed, the Fourier coefficients of the hole concentration are the reciprocal of b_k in accordance with the mass-action law. Fourier coefficients a_{dk} and a_{ak} are found from the system similar to Eq. (5) for each impurity species. If, however, the assumption of negligible minority carrier capture and emission rates is not satisfied, such as for gold in silicon,¹⁴ the complete rate Eqs. (3) should be used instead of Eq. (4). The system of equations for a_k then becomes somewhat more complicated than Eq. (5)

$$a_k(i\omega k + \tau^{-1}) + \sum_{m=-\infty, m \neq k}^{\infty} a_m (C_n n_0 b_{k-m} + C_p p_0 b_{k-m}^{-1}) = 0, \quad k \neq 0, \quad (10a)$$

$$a_0 \tau^{-1} + \sum_{m=-\infty, m \neq 0}^{\infty} a_m (C_n n_0 b_{-m} + C_p p_0 b_{-m}^{-1}) = \left(e_n + C_p \frac{p_0}{b_0} \right) \frac{N}{N_0^+}, \quad (10b)$$

where the impurity time constant is now defined as $\tau = (e_n + C_n n_0 b_0 + e_p + C_p p_0 b_0^{-1})^{-1}$. It should be noted, however, that in wide band-gap semiconductors, such as SiC or GaN, where the described impurity ionization effects are not negligible at room temperature, the minority carrier concentration is usually extremely small in the semiconductor bulk and is small for moderate reverse bias in the junction depletion region. Additionally, even relatively deep impurities in wide band-gap semiconductors are often much closer to one of the allowed energy bands than to the other, so that minority capture and emission rates are expected to be much smaller than the corresponding majority capture and emission rates. Therefore, all terms including minority carrier concentration and capture and emission rates can usually be omitted without sacrificing accuracy and Eqs. (9) and (10) reduce to the simplified Eqs. (5) and (7).

III. INFLUENCE OF AC BIAS AMPLITUDE ON JUNCTION ADMITTANCE

We use the developed general admittance model to find the behavior of the Schottky junction admittance for different ac bias amplitudes ranging from the values at which the small-signal condition is satisfied to the ones which significantly exceed the value of $k_B T/q$. Admittance is calculated as a function of temperature and as a function of ac bias frequency at room temperature. As an object for calculations we chose 6H-SiC Schottky diodes. As we have already mentioned, in this material all technologically important impurities are relatively deep and thus incompletely ionized even at room temperature. We do the calculations for the nitrogen donors which are the shallowest of the SiC doping impurities and for the boron acceptors which are the deepest ones. In the case of nitrogen, the probabilities of occupation of the hexagonal (ionization energy 81 meV) and quasicubic lattice sites (ionization energies 137.6 and 142.4 meV)²¹ are assumed to be equal. Additionally, since the ionization energies of nitrogen on two quasicubic sites are very close, these two sites were modeled by a single site with the ionization energy of 140 meV and the concentration of twice that of each single site. In the case of boron, the ionization energies of the different lattice sites are not known, so in calculations a single boron level at 0.3 eV above the valence band was used.²¹

The bulk value of the Fermi level was calculated from the charge neutrality equation, which for the case of two nitrogen levels is

$$N_c e^{-(E_c - \mu_F)/k_B T} = \frac{N_1}{1 + \gamma_1 e^{-(E_1 - \mu_F)/k_B T}} + \frac{N_2}{1 + \gamma_2 e^{-(E_2 - \mu_F)/k_B T}}, \quad (11)$$

where E_1 , E_2 , N_1 , N_2 , and γ_1 , γ_2 are ionization energies, concentrations, and degeneracy factors of the first and second impurity levels, respectively. The free-electron distribution is assumed to be nondegenerate, and the minority carrier concentration is assumed to be negligible. After finding the Fermi level, the free-carrier concentration and its Fourier coefficients are found using Boltzmann's statistics and formula (6). Minority carrier trapping effects are neglected, and Fourier coefficients a_k of the ionized impurity concentration are found by numerically solving the system (5) using the Gaussian elimination with partial pivoting method. Fourier coefficients of the potential are found by solving the system of Eqs. (9) self-consistently with the system (5), using an adaptive finite-difference method. Junction admittance is then found using formula (1). Impurity ionization time constant, which enters the system (5) is, in general, potential dependent. The influence of the electric field on the emission rate (the Poole-Frenkel effect) can be taken into account using the following expression:²⁰

$$e = e_0 \left[\frac{(x-1)\exp(x)+1}{x^2} + \frac{1}{2} \right], \quad (12)$$

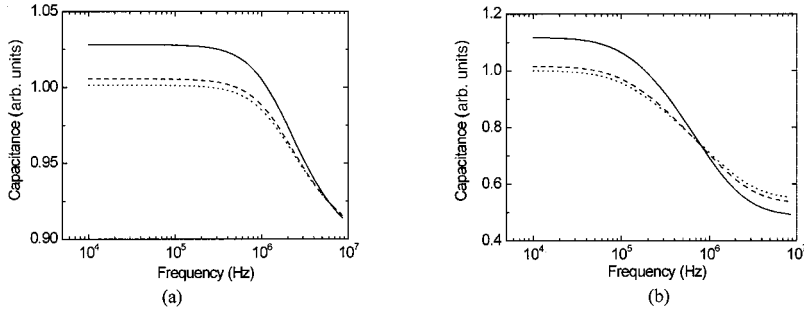


FIG. 1. Capacitance of (a) N-doped and (b) B-doped 6H-SiC Schottky junction as a function of measurement ac signal frequency calculated for different ac bias amplitudes: 30 mV (dotted line), 60 mV (dashed line), and 150 mV (solid line). Capacitance is normalized by its small-signal low-frequency value.

where $x = \beta^{-1} \sqrt{Eq/\pi\epsilon}$, E is the local electric field and e_0 is the zero field-emission rate, which for donorlike impurities is given by

$$e_0 = C_n N_c \exp(-E_D/k_B T)/\gamma.$$

Figure 1 represents room-temperature frequency dependencies of the Schottky junction capacitance for different ac bias amplitudes in the case of nitrogen-doped 6H-SiC with the concentration of nitrogen atoms of 10^{18} cm^{-3} (a) and in the case of boron-doped SiC with the concentration of 10^{16} cm^{-3} (b). The condition for the small-signal model to be valid is $\varphi_1 \ll k_B T/q$. However, since the junction admittance is defined by carrier sweep out and impurity ionization in the depletion region tail, the ac potential in this region is smaller than at the metal-semiconductor interface. Consequently, in these examples, the junction capacitance begins to deviate from its small-signal limit for ac bias voltages larger than $k_B T/q$, which at room temperature is equal to approximately 26 mV.

The two components of the junction current contribute differently to the current harmonic content. The degree of distortion of the free-carrier component of the junction current is not large since the carrier sweep out takes place in a small part of the depletion region tail close to the semiconductor bulk region, where the ac potential is small even for a relatively large applied ac bias. On the other hand, the junction current component caused by impurity ionization may be distorted more noticeably because the ionization processes take place deeper in the space-charge region,²² where the ac potential amplitude is larger. Therefore, the difference between the small- and large-signal admittance values is expected to be larger in the case of deeper impurities with a larger degree of carrier freeze out, such as boron acceptors in this example. The low-frequency capacitance increases with increasing the ac bias because more charge can be released from the impurities by larger potential changes (this charge is limited by the number of unionized atoms). On the contrary, the high-frequency value of the capacitance is determined only by the free carriers, and for larger ac potentials a larger fraction of them respond on frequencies other than the fundamental, thus decreasing the measured capacitance value.

The temperature dependence of the junction conductance for 1 MHz ac bias with different amplitudes was calculated and is represented in Fig. 2. The conductance goes through a peak when the inverse of the effective, i.e., averaged over the space-charge region, impurity ionization time constant is approximately equal to the measurement signal circular fre-

quency. The junction potential distribution affects the free-carrier and ionized impurity distributions, which leads to the dependence of the effective impurity time constant and conductance peak position on the ac bias amplitude. One consequence of this is that admittance spectroscopy data analysis, which relies on the relationship between the measurement signal frequency and the impurity time constant, should in general be performed using a large-signal admittance model.

In a recent paper,²³ we experimentally confirmed the influence of the junction potential distribution on the impurity ionization time constant. We have shown that at low temperatures an admittance spectroscopy Arrhenius plot cannot be approximated accurately by the curve calculated using a small-signal model because the ac potential becomes large compared to $k_B T/q$. On the other hand, the admittance calculated using our general model fit the experimental data well across our entire measurement temperature range.

IV. LOW-TEMPERATURE ADMITTANCE DATA: COMPARISON WITH THE LARGE- AND SMALL-SIGNAL MODELS

Here we present experimental data for 6H-SiC Schottky diode admittance as a function of temperature fitted using the method of least squares with our general junction admittance model and, for comparison, with the small-signal model.⁶ The diodes were fabricated in a lift-off process using aluminum as a contact metal. To minimize the influence of device series resistance on the admittance measurements diodes

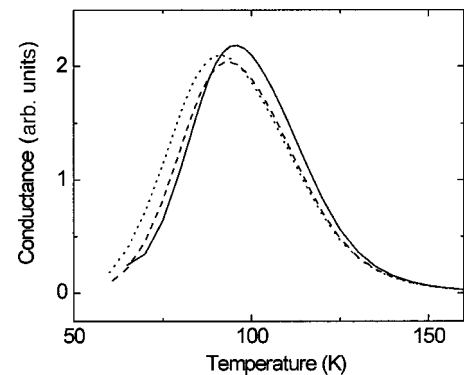


FIG. 2. Calculated conductance of B-doped SiC Schottky junction as a function of temperature for 1 MHz measurement signal frequency at different ac signal amplitudes: 30 mV (dotted line), 60 mV (dashed line), and 150 mV (solid line).

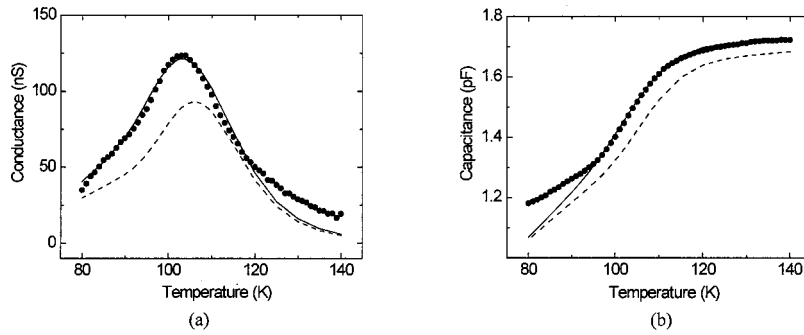


FIG. 3. Least-squares fit of the general admittance model (solid line) to 100 kHz admittance data for N -doped SiC Schottky diode and a least-squares fit using the small-signal model (dashed line).

with the smallest areas that still provided acceptable measurement signal-noise ratio were chosen. The measurements were performed in the Janis SVT-300 liquid-nitrogen cryostat using Hewlett Packard HP 4275A multifrequency LCR meter. The measurements were done at the frequency of 100 kHz in the temperature range of 80–140 K with the measurement ac signal rms value set to 30 mV. Under these conditions the ac bias amplitude is about five times larger than $k_B T/q$ at 100 K, so that the small-signal condition is invalid in the entire measurement temperature range, and a large-signal model is expected to be more accurate than the small-signal model.

The data and fitting results are presented on Fig. 3. It was not possible to obtain a satisfactory least-squares fit to the experimental data assuming a single dominant impurity level, which means that several impurities in this sample have approximately the same ionization time constants, and the conductance peak is a superposition of the peaks corresponding to these impurities. A good fit was obtained when capture cross sections of two nitrogen levels with activation energies of 0.081 and 0.14 eV were used as the fitting parameters. Additionally, it was found that to obtain a satisfactory correspondence between the calculated admittance and experimental data, the Poole-Frenkel effect had to be taken into account, which was done using Eq. (12). As can be seen from Fig. 3, a satisfactory fit could not be obtained using the small-signal junction admittance model, illustrating the failure of the small-signal approximation under these experimental conditions.

The conductance calculated from the general model fits experimental data well in the temperature range of 80–120 K, including the conductance “hump” at 80–90 K, which is due to nitrogen on the hexagonal site. In contrast to the theoretical curve, the experimental conductance data does not go to zero at temperatures above 120 K. This difference can be explained by the influence of another impurity. The calculated junction capacitance fits the experimental data very well at temperatures above 95 K but deviates from it at lower temperatures. At these temperatures, the junction depletion region expands up to the diode contacts, and the measured capacitance begins to saturate at its lowest value determined by the Schottky and return contacts mutual geometry. This geometrical effect was not taken into account in the calculations, so unlike the experimental data, the calculated capacitance drops to zero in the low-temperature limit. The nitrogen donor capture cross sections determined from the fitting procedure are $\sigma_1 = 9.6 \times 10^{-17} \text{ cm}^2$ for the hexagonal lattice

site and $\sigma_2 = 2.1 \times 10^{-15} \text{ cm}^2$ for the quasicubic sites, which agree with the data reported in literature.²¹

V. SUMMARY

We have created a general reverse bias Schottky junction admittance model, which is valid in a broader range of temperatures and bias amplitudes than the small-signal admittance models. The model is not based on the small-signal approximation, and thus takes into account large-signal effects which are present for large ac bias amplitudes and at low temperatures when the ac potential is comparable to or larger than $k_B T/q$. The model also takes into account incomplete impurity ionization.

The model allows calculation of the junction potential and current harmonics for an arbitrary periodic excitation, thus allowing calculation of the junction transfer function and, as a particular case, the junction admittance. Because the small-signal assumption is not used, the ionized impurity and free-carrier concentration changes are not treated as proportional to bias changes. Fourier coefficients of the ionized impurity concentration are found from a system of linear equations for each impurity species. It is assumed that the free-carrier relaxation time is short compared to the bias period, so that the free-carrier distribution is near equilibrium. Fourier coefficients of the free-carrier concentration are thus found using the Fermi or Boltzmann statistics. Junction potential is then found by solving the system of differential equations for each potential harmonic self consistently with the equations for ionized impurity and free-carrier concentrations. In the small-signal limiting case our model reduces to the general small-signal model given in Ref. 6.

The general model predicts the junction admittance to deviate from the values given by the small-signal model with the deviation being stronger at lower temperatures or larger ac bias amplitudes, and for deeper impurities with a larger degree of carrier freeze out. The model has been used for admittance spectroscopy data analysis and provided an improved value for the activation energy of nitrogen donors in 6H-SiC.²³ We also performed a least-squares fit of the junction admittance as a function of temperature for N -doped SiC in the temperature range where the applied ac bias is larger than $k_B T/q$. The model describes the junction admittance more accurately than the small-signal model, resulting in a better correspondence between the theoretical and the experimental data.

The general admittance model may be useful in all cases

where the reverse biased semiconductor junction is used or modeled as an impedance device under periodic bias excitation with amplitude larger than the thermal potential $k_B T/q$. This may occur, for instance, for diodes working as variable capacitors in ac signal circuits. Another possible application is for electronic devices working at low temperatures where the small-signal condition is not satisfied even for relatively small ac biases. Additionally, at low temperatures, impurities completely ionized at room temperature may be in a partial carrier freeze out, which is also accounted for in the model.

This is possible in the wide band-gap semiconductors such as SiC and GaN even at relatively high temperatures. In all these cases the developed model should provide a more accurate device description compared to the traditional small-signal models.

ACKNOWLEDGMENT

This work was supported by the Office of Naval Research, Dr. C. Wood program manager.

*Electronic address: AVL1@ECE.MSState.EDU

¹W. Schottky, *Z. Phys.* **113**, 367 (1939).

²W. Schottky, *Z. Phys.* **118**, 539 (1942).

³B. M. Vul and E. I. Zavaritskaya, *Zh. Eksp. Teor. Fiz.* **38**, 10 (1960) [*Sov. Phys. JETP* **11**, 6 (1960)].

⁴C. T. Sah and V. G. K. Reddi, *IEEE Trans. Electron Devices* **11**, 345 (1964).

⁵G. I. Roberts and C. R. Crowell, *Solid-State Electron.* **16**, 29 (1973).

⁶D. L. Losee, *J. Appl. Phys.* **46**, 2204 (1975).

⁷W. G. Oldham and S. S. Naik, *Solid-State Electron.* **15**, 1085 (1972).

⁸G. Vincent, D. Bois, and P. Pinard, *J. Appl. Phys.* **46**, 5173 (1975).

⁹B. M. Vul, *Dokl. Akad. Nauk SSSR* **129**, 61 (1959) [*Sov. Phys. Dokl.* **4**, 1246 (1960)].

¹⁰G. I. Roberts and C. R. Crowell, *J. Appl. Phys.* **41**, 1767 (1970).

¹¹W. Shockley and W. T. Read, Jr., *Phys. Rev.* **87**, 835 (1952).

¹²R. N. Hall, *Phys. Rev.* **87**, 387 (1952).

¹³V. I. Perel and A. L. Efros, *Fiz. Tekh. Poluprovod* **1**, 1963 (1967) [*Sov. Phys. Semiconductors* **1**, 1403 (1968)].

¹⁴L. Forbes and C. T. Sah, *IEEE Trans. Electron Devices* **ED-16**, 1036 (1969).

¹⁵M. Beguwala and C. R. Crowell, *Solid-State Electron.* **17**, 203 (1974).

¹⁶P. Frandon and J.-C. Hoffmann, *C R. Acad. Sci.* **258**, 1749 (1964).

¹⁷P. Frandon and J.-C. Hoffmann, *C R. Acad. Sci.* **258**, 5371 (1964).

¹⁸P. Frandon and J.-C. Hoffmann, *C R. Acad. Sci.* **259**, 2377 (1964).

¹⁹Hewlett Packard HP4280A C Meter/C-V plotter operation and service manual.

²⁰J. L. Hartke, *J. Appl. Phys.* **39**, 4871 (1968).

²¹A. V. Los and M. S. Mazzola, *J. Electron. Mater.* **30**, 235 (2001).

²²Fermi distribution is most susceptible to potential changes at the point where the impurity energy level intersects the corresponding quasi-Fermi level. The ionization processes therefore take place mostly around this point. Position of this intersection point in the space-charge region is defined by the impurity activation energy, concentration, and junction potential.

²³A. V. Los and M. S. Mazzola, *J. Appl. Phys.* **89**, 3999 (2001).