Numerical Parameterization of Chemical-Vapor-Deposited (CVD) Single-Crystal Diamond for Device Simulation and Analysis

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Abstract—High-quality electronic-grade intrinsic chemical-vapor-deposited (CVD) single-crystal diamond layers having exceptionally high carrier mobilities have been reported by Isberg *et al.* This makes the realization of novel electronic devices in diamond, particularly for high-voltage and high-temperature applications, a viable proposition. As such, models which can capture the particular features of diamond as a semiconductor are required to analyze, optimize, and quantitatively design new devices. For example, the incomplete ionization of boron in diamond and the transition to metallic conduction in heavily boron-doped layers require accurate carrier freeze-out models to be included in the simulation of diamond devices. Models describing these phenomena are proposed in this paper and include numerical approximation of intrinsic diamond which is necessary to formulate doping- and temperature-dependent mobility models. They enable a concise numerical description of single-crystal diamond which agrees with data obtained from material characterization. The models are verified by application to new Schottky m-i-p⁺ diode structures in diamond. Simulated forward characteristics show excellent correlation with experimental measurements. In spite of the lack of impact ionization data for single-crystal diamond, approximation of avalanche coefficient parameters from other wide-bandgap semiconductors has also enabled the reverse blocking characteristics of diamond diodes to be simulated. Acceptable agreement with breakdown voltage from experimental devices made with presently available single-crystal CVD diamond is obtained.

Index Terms—Diamond, numerical parameterisation, Schottky diodes, semiconductor device modeling.

I. INTRODUCTION

AS THE demand for the voltage and power ratings of solid-state switching devices increases, conventional silicon technology has fundamental physical limitations when higher current densities and blocking voltages are required. Additionally, the need for more robust devices which are capable of operation in harsh conditions has led to the exploration of wide-bandgap materials as alternatives to silicon. Diamond has been described as the “ultimate wide-bandgap material” due to its extreme material properties. Recent advances in synthesizing high-quality single-crystal chemical-vapor-deposited (CVD) intrinsic diamond films have enabled the observation of extremely desirable electronic properties [1]–[3]. Some of these are given in Table I for diamond and other wide-bandgap materials that are currently being considered for electronic devices.

The exceptionally high intrinsic carrier mobilities of up to 3800 and 4500 cm²/V · s in single-crystal diamond (for holes and electrons, respectively) can only be exploited if an undoped region is present in the main conduction path. This points to the need for a more creative approach to control carrier injection into an intrinsic region to fully harness the ultrahigh-mobility properties of diamond. However, due to the limited amount of data which has been obtained from this relatively new CVD material, numerical analysis in tools (such as the 2-D physics-based device simulator MEDICI), essential for the design and analysis of power devices, cannot be used to correctly simulate the performance of diamond devices due to the lack of appropriate physical model parameters.

Physical models which have to be specially formulated for single-crystal diamond are proposed in this paper and include the incomplete ionization of boron, completely intrinsic carrier-free material, dependences of carrier transport on doping and temperature (highlighting both individual concentration and mobility dependence on temperature), and impact ionization during avalanche breakdown. Verification of this numerical description of diamond is obtained through comparison of simulated and experimental device characteristics of Schottky m-i-p⁺ diodes.

II. DEVICE UNDER INVESTIGATION

The Schottky m-i-p⁺ diode has a relatively simple layered structure with potential for use as a high-voltage unipolar diode

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TABLE I
ELECTRICAL PROPERTIES OF COMMON WIDE-BANDGAP SEMICONDUCTORS COMPARED TO SILICON

	Si	GaAs	4H-SiC	6H-SiC	GaN	Diamond
Bandgap (eV)	1.12	1.424	3.26	3.03	3.295	5.47
Maximum Electric Field (MV/cm)	0.41	0.48	2.4	2.4	5	20
Electron Mobility ($\text{cm}^2/\text{V}\cdot\text{s}$)	1450	8600	900	400	2000	4500
Hole Mobility ($\text{cm}^2/\text{V}\cdot\text{s}$)	480	130	120	100	200	3800
Saturation Velocity (cm/s) $\times 10^7$	0.86	0.72	2	2	2.5	2.7
Thermal Conductivity (W/m-K)	1.5	0.46	4.9	4.9	1.3	20
Relative Dielectric Constant	11.7	12.9	10	9.7	5.35	5.7
Substrate Diameter (mm)	200	150	75	75	75	5
<i>Figures of Merit (relative to Si)</i>						
Johnson's [†]	1.00	7.11	178	256	1740	32400
Keyes' [‡]	1.00	0.43	4.62	4.62	1.37	21.9
Baliga's [*]	1.00	15.3	156	116	2900	444000

[†] Johnson's figure of merit estimates the potential of a material for high frequency and high power applications.

[‡] Keyes' figure of merit has its relevance in integrated circuit design, and limits the current flowing in a integrated circuit and the heat dissipated as a result of this current.

^{*} Baliga's figure of merit is a measure of the specific on-resistance of the drift region of a vertical power transistor [24].

Fig. 1. Fabricated Schottky m-i-p⁺ diode used to ascertain the applicability of the material models derived for intrinsic and boron-doped single-crystal diamond. Numerical implementation of the device structure is also shown alongside the fabricated device.

to replace Si p-i-n diodes in power electronic systems. It is also a good trial structure for the analysis and correlation of numerical and experimental device characteristics in order to determine the suitability of material models specific to single-crystal diamond. The vertical device consists ideally of a completely intrinsic (i) diamond layer of thickness L_I grown on a 300–600- μm -thick highly boron-doped p⁺ diamond substrate with concentration $N_A(p^+) > 2.0 \times 10^{19} \text{ cm}^{-3}$, as shown in Fig. 1. On the i-layer, a cathode comprising of a Schottky metal

[aluminum (Al) or gold (Au)] is deposited, while a titanium–Al ohmic stack is used as the anode contact.

One characteristic of the diamond surface is that its electron affinity depends highly on the nature of the surface termination. In the experimental devices, all diamond surfaces were treated with an oxygen plasma prior to contact deposition resulting in an electron affinity χ of 1.3 eV [4]. The nature of this surface treatment affects the potential barrier ϕ_{Bp} and, hence, the turn-on voltage V_{TO} of the Schottky m-i-p⁺ diode.

III. MATERIAL MODELS

A. Incomplete Ionization of Dopants

Activation of dopants is an important issue that specifically plagues the fabrication of diamond electronic devices. The problem of dopant activation originates from the wide 5.47-eV bandgap of diamond and the large ionization energies of dopants in the material. Phosphorus and boron are known donor and acceptor species in diamond and exhibit activation energies ΔE_{An} and ΔE_{Ap} of 590 and 360 meV, respectively [5], [6]. The larger ΔE_{An} of phosphorus results in insufficient carrier activation at room temperature for effective control of resistivity with n-doped layers. Boron-doped diamond also suffers from the same problem, albeit to a less severe extent, and can be used for some resistivity control through p-type doping.

However, incomplete ionization still limits the number of carriers which can be introduced into the valance band with increasing boron concentrations. Controlled doping is limited to hole concentrations of 10^{16} cm^{-3} with boron concentrations of $3.0 \times 10^{19} \text{ cm}^{-3}$. When the boron concentration exceeds this value, an impurity band which overlaps with the diamond valance band is formed. Under these conditions, the diamond starts to exhibit metallic, rather than semiconducting, conduction properties. Therefore, it is possible to achieve metallic conduction layers with p^+ characteristics and hole concentrations in excess of 10^{19} cm^{-3} with very high concentration of boron in diamond.

In the m-i- p^+ diode structure, a highly boron-doped p^+ layer is used as a hole injector into the i-layer under forward-bias conditions. This enables the voltage-blocking layer, under reverse bias, to be a thin undoped i-layer. It also allows for the ultrahigh mobility of diamond in the i-layer (see Table I) to be exploited during space-charge-limited (SCL) conduction in the forward direction [2], [7].

Additionally, the ionization of intrinsic nitrogen impurities that result during CVD single-crystal diamond growth [8] must be considered, as these serve as compensating donor species. It can be shown that the hole concentration p in the material is

$$p = \frac{1}{2} Q_{p(\text{net})} + \sqrt{\frac{1}{4} Q_{p(\text{net})}^2 + n_i^2} \quad (1)$$

where n_i is the intrinsic carrier concentration of diamond, and $Q_{p(\text{net})}$ is the net carrier concentration that takes into account the degree of compensation from nitrogen impurities of concentration N_D , which is given by

$$Q_{p(\text{net})} = -\frac{1}{2} (N_A^* + N_D) + \sqrt{\frac{1}{4} (N_A^* + N_D)^2 + N_A^* (N_A - N_D)} \quad (2)$$

where N_A and N_A^* are the doped (chemical) and activated boron concentration, respectively [9], of which the latter is given by

$$N_A^* = \frac{N_V}{g_a} \exp \left[-\frac{\Delta E_A(N_A, T)}{kT} \right] \quad (3)$$

Fig. 2. Band structure of doped single-crystal diamond (shown here with respect to a Schottky m-i- p^+ diode structure) at zero bias.

with a degeneracy factor g_a of four. N_V and k are the density of states at the valance band edge and the Boltzmann constant, respectively. Note that the ΔE_{Ap} of boron is a function of both temperature and doping and can be modeled by the extended Pearson and Bardeen approximation for carrier freeze-out [10]

$$\Delta E_{Ap}(N_A, T) = E_{Ap0} - \alpha_1 N_A^{\frac{1}{3}} + \beta_1 (T^{-\gamma_1} - 300^{-\gamma_1}) \quad (4)$$

where E_{Ap0} , α_1 , β_1 , and γ_1 have values of 360 meV, $3.037 \times 10^{-8} \text{ cm}$, 200, and 0.95, respectively [11]. The calculation of ionized impurity concentration in (3) hence takes into account the enhanced activation of boron atoms due to the reduction in ΔE_{Ap} with increasing temperature, as given in (4).

Incomplete ionization of boron in single-crystal diamond has been shown to be less of an issue for boron concentrations in excess of $3.0 \times 10^{19} \text{ cm}^{-3}$ [6]. For p^+ diamond layers, a metallic-type conduction mechanism dominates for boron concentrations in excess of $3.0 \times 10^{20} \text{ cm}^{-3}$ due to overlapping of the acceptor and valance bands at high doping concentrations, where ΔE_{Ap} reduces to zero with increasing N_A . Hopping conduction results between regions of incomplete ionization and metallic conduction, where the acceptor band thins and enables carriers to transit from the acceptor level E_a to the valance band E_v , as shown in Fig. 2 for a diamond Schottky m-i- p^+ diode. This transition region is observed as a nonlinear decrease in resistivity of boron-doped single-crystal diamond layers with increasing N_A (beyond 10^{19} cm^{-3}) [6], [12] and has been numerically modeled as a linear transition to complete ionization with parameters α_{hop} and β_{hop} (taking values of 1.11 and $3.0 \times 10^{19} \text{ cm}^{-3}$, respectively) [13].

Equation (5), shown at the bottom of the next page, thus completely describes the various degrees of incomplete ionization of boron in single-crystal diamond layers (band, hopping, and metallic conduction) and thus relates the hole concentration p to the chemical concentration of boron N_A . This $p \propto N_A$ relation is shown in Fig. 3.

Fig. 3. Incomplete ionization model implemented for boron in synthetic single-crystal diamond, shown with varying degrees of nitrogen compensation N_D .

B. Numerical Approximation of Intrinsic Material

The incorporation of completely intrinsic layers in CVD single-crystal diamond device design leads to issues with regard to numerical analysis of devices, as the carrier concentration in these intrinsic layers n_i is on the order of 10^{-27} cm^{-3} at 300 K. This excessively low carrier number necessitates the numerical approximation of carrier-free diamond layers with layers of an effective quasi-doping $N_A(i')$ so as to facilitate numerical analysis. On the other hand, it is important that this concentration does not result in a deviation of the numerically implemented device from the physical device performance.

In the case of the Schottky m-i-p⁺ diode, the quasi-doping $N_A(i')$ must be such that, at zero bias, the ϕ_{Bp} resulting from the Schottky electrode results in the formation of a depletion region under the cathode which extends all the way to the p⁺ substrate. This ensures that the resulting quasi-intrinsic layer exhibits SCL current conduction when forward biased. Preliminary investigations of a 10- μm diamond-Au Schottky m-i-p⁺ diode have revealed that for $N_A(i') \leq 10^{11} \text{ cm}^{-3}$, numerical and experimental characteristics match with an error of less than 10%. Further reduction of $N_A(i')$ gives little change in device characteristics for anode biases V_A of 2 V in excess of the turn-on voltage V_{TO} . This indicates that the current conduction mechanism for $N_A(i') \leq 10^{11} \text{ cm}^{-3}$ is completely SCL and not influenced by bulk conduction. Thus, intrinsic CVD diamond can be represented as quasi-intrinsic with concentrations of $N_A(i') = 10^{11} \text{ cm}^{-3}$ (the highest effective

doping allowable without incurring problems of “zero” carriers in simulation).

C. Carrier Mobility Dependences

Concentration-dependent Hall and time-of-flight (TOF) hole mobility μ_p values reported [6], [14] for heavily boron-doped p⁺ diamond (with $N_A > 10^{14} \text{ cm}^{-3}$) are shown graphically in Fig. 4. Also shown in the figure is the high hole mobility of $3800 \text{ cm}^2/\text{V} \cdot \text{s}$ for intrinsic CVD single-crystal diamond [1]–[3] implemented at the numerical intrinsic approximation $N_A(i')$. Coupling the Hall and TOF mobility data in both single-crystal i and p⁺ diamond with intermediate values reported in the literature, it is possible to formulate a concise concentration-dependent mobility model for boron-doped homoepitaxial diamond.

A widely used empirical expression for modeling the doping dependence of mobility $\mu_p(N_A)$ is

$$\mu_p(N_A) = \mu_0 \exp\left(-\frac{p_c}{N_A}\right) + \frac{\mu_{\max} - \mu_0}{1 + (N_A/C_r)^{\alpha_2}} - \frac{\mu_1}{1 + (C_s/N_A)^{\beta_2}} \quad (6)$$

where the terms μ_0 , μ_1 , $\mu_{\max}$, p_c , C_r , C_s , α_2 , and β_2 are fitting factors to existing mobility data [15]. Equation (6) has been used extensively to model hole and electron mobility variations

$$p = \begin{cases} \frac{1}{2}Q_{p(\text{net})} + \sqrt{\frac{1}{4}Q_{p(\text{net})}^2 + n_i^2}, & \text{for } N_A < 3 \times 10^{19} \text{ cm}^{-3} \\ \alpha_{\text{hop}}N_A - \beta_{\text{hop}}, & 3 \times 10^{19} \leq N_A \leq 3 \times 10^{20} \text{ cm}^{-3} \\ N_A, & N_A > 3 \times 10^{20} \text{ cm}^{-3} \end{cases} \quad (5)$$

Fig. 4. Concentration-dependent mobility model for homoepitaxial boron-doped diamond layers. $\mu_p(N_A)$ variations for boron-doped silicon and aluminum-doped 4H-SiC are also shown for comparison [17], [18]. Numerical implementation of (6) via table lookup array (required by MEDICI) is shown as square data points in the figure [13].

TABLE II
CONCENTRATION-DEPENDENT MOBILITY MODEL $\mu_p(N_A)$ PARAMETERS FOR P-TYPE SEMICONDUCTING MATERIALS

Material	Si [†]	4H-SiC [‡]	Diamond
μ_0 (cm ² /V-s)	44.9	40	105
$\mu_{\max}$ (cm ² /V-s)	470.5	950	3815
μ_1 (cm ² /V-s)	29.0	0	50
C_r (cm ⁻³)	2.23×10^{17}	2×10^{17}	10^{14}
C_s (cm ⁻³)	6.10×10^{20}	0	10^{14}
α_2	0.719	0.76	0.61
β_2	2.0	0	5.0
p_c (cm ⁻³)	9.23×10^{16}	0	0

[†] after Masetti *et al.* for boron-doped Si [17].

[‡] after Schaffer *et al.* for aluminium-doped 4H-SiC [18].

with doping in materials such as silicon and silicon carbide [16]–[18]. Fitting parameters for these materials are shown in Table II for boron and aluminum doping, respectively. By incorporating $N_A(i')$, we have developed a concentration-dependent mobility model for intrinsic and boron-doped single-crystal diamond layers, consistent with experimentally observed Hall and TOF hole mobility data. This $\mu_p(N_A)$ model for CVD diamond is also shown in Fig. 4, the parameters of which are listed in Table II. From the mobility plot, it can be seen that while the hole mobilities for both Si and SiC stay relatively constant at their respective peak values for a wide range of doping concentrations up to 10^{16} and 10^{17} cm⁻³, respectively, the high-hole-mobility $\mu_p(i)$ seen in i-diamond rapidly reduces to only 1.5% of its intrinsic value over the doping range of $10^{12} < N_A < 10^{16}$ cm⁻³. This reinforces the advantages of using intrinsic layers in diamond high-voltage power devices for achieving high current densities by exploiting ultrahigh

mobility while preserving the high breakdown capability of the intrinsic material to optimize the reverse blocking performance of such devices.

In addition to doping-dependent carrier transport, it is necessary to model mobility variations at elevated (junction) temperatures resulting from harsh device operating conditions where lattice and ionized impurity scattering mechanisms cannot be neglected, particularly in heavily doped semiconducting materials. For intrinsic CVD single-crystal diamond layers, Isberg *et al.* [19] have recently extracted from drift mobility measurements a $\mu_p(i)(T) \propto T^S$ dependence, where $S \approx -1.55$ for $T < 343$ K attributed to acoustic phonon scattering, and a steeper $S \approx -3.4$ dependence for higher temperatures in excess of 343 K, as shown in Fig. 5.

However, the presence of boron atoms within the diamond lattice complicates the analysis. The hole mobility in p⁺-type material exhibits a positive temperature coefficient at

Fig. 5. Temperature-dependent mobility for intrinsic and heavily doped p^+ diamond layers.

low temperatures, unlike most other wide-bandgap semiconductors. Somogyi [20] advocates the use of Brooks–Herring and Conwell–Weisskopf mobility approximations to model this behavior in highly boron-doped monocrystalline synthetic diamond, where the power law dependence used to take into account ionized impurity scattering at low temperatures is $S \approx 2.5$, changing to $S \approx -3$ at high temperatures due to lattice scattering effects. The former is specific to doped p^+ diamond and is based on the scattering electrostatic Coulomb forces that arise due to the attenuation of ionized impurities with temperature through increasing lattice vibrations at higher temperatures. This characteristic is thought to be seen in single-crystal diamond due to the large ΔE_{Ap} of boron impurities in the material [20]–[22]. The boundary between these two conduction regimes is characterized by a temperature at which the hole mobility is a maximum $T_{\max}$. It has been empirically shown [23] that for $N_A > 10^{18} \text{ cm}^{-3}$, $T_{\max}$ is in excess of 600 K, and hence, in this paper, we use $\mu_p(p^+)(T) \propto T^{2.5}$, as shown in Fig. 5, limited to $T \leq 600 \text{ K}$, where carrier transport is dominated primarily by ionized impurity scattering.

Incorporating these thermal mobility trends into the concentration-dependent mobility relation in (6), it is possible to obtain a unified description of carrier transport

$$\mu_p(N_A, T) = \mu_{\min}(T) + \frac{\mu_{\max}(T) - \mu_{\min}(T)}{1 + \left(\frac{T}{300}\right)^{m_1} \left(\frac{N_A}{C_0}\right)^{\gamma_2}} \quad (7)$$

where

$$\mu_{\min, \max}(T) = \mu_{\min 0, \max 0} \left(\frac{T}{300}\right)^{n_{\min, \max}} \quad (8)$$

in which the coefficients $\mu_{\min 0}$, $\mu_{\max 0}$, $n_{\min}$, $n_{\max}$, m_1 , C_0 , and γ_2 are material-specific fitting parameters required to allow for variations in hole mobility in both intrinsic and heav-

ily boron-doped single-crystal diamond layers. Temperature-range-specific implementation of the $\mu_p(T)$ relations obtained empirically [20] and experimentally [19], [23] leads to (7) and (8) being a unified description of doping- and temperature-dependent carrier transport $\mu_p(N_A, T)$ in single-crystal diamond. These are shown graphically in Fig. 6, the coefficients of which are given in Table III. $\mu_p(N_A, T)$ includes hole mobility dependences on both doping and temperature in its description and is used in the discussions that follow.

D. Impact Ionization Coefficients

The susceptibility of carrier transport to variations in doping and temperature is important for accurately predicting the “on” characteristics of diamond devices. However, of equal importance in power device design are the impact ionization integral coefficients α_n and α_p for electrons and holes, respectively. Under heavy reverse bias, the increase of the ionization integral toward unity indicates the onset of avalanche carrier generation due to impact ionization [24], thus resulting in device breakdown. The characterization of the breakdown voltage V_{BR} is an important parameter in high-voltage device design so as to have a clear understanding of the static voltage blocking capability of these devices. It can be shown [25], [26] that

$$\alpha_{n,p} = A_{n,p} \exp\left(-\frac{B_{n,p}}{\xi}\right)^{c_{n,p}} \quad (9)$$

in which $A_{n,p}$, $B_{n,p}$, and $c_{n,p}$ are fitting parameters and ξ is the lateral electric field through the semiconductor layer. However, no information on these coefficient parameters is presently available in the literature for single-crystal diamond [27]. Thus, at the current stage of diamond device technology, in order to approximately quantify the blocking capability of diamond power devices in reverse bias, estimated values

Fig. 6. Unified hole mobility $\mu_p(N_A, T)$ implemented for CVD single-crystal diamond showing good correlation with data and predictions previously reported [6], [19], [20], [23].

TABLE III
PARAMETERS DESCRIBING THE UNIFIED HOLE MOBILITY IN SINGLE-CRYSTAL DIAMOND

Parameter	Coefficient Value*	
	$T \leq 343$ K	$343 < T < 600$
$\mu_{\max 0}$ (cm ² /V-s)	3443	4399
$n_{\max}$	-1.55	-3.4
$\mu_{\min 0}$ (cm ² /V-s)	55	
$n_{\min}$	2.5	
m_1	-2	
C_0 (cm ⁻³)	1.12×10^{14}	
γ_2	0.589	

* In this approximation [20,23], p^+ diamond is taken as material with $N_A \geq 10^{18}$ cm⁻³.

TABLE IV
IMPACT IONIZATION COEFFICIENT PARAMETERS OF SELECTED SEMICONDUCTORS

Material	Si [†]	4H-SiC [‡]	Diamond
Bandgap (eV)	1.12	3.26	5.47
A_n (cm ⁻¹)	7.030×10^5	4.50×10^5	1.89×10^5
A_p (cm ⁻¹)	1.582×10^6	3.50×10^6	5.48×10^6
B_n (V/cm)	1.231×10^6	9.00×10^6	1.70×10^7
B_p (V/cm)	2.036×10^6	8.00×10^6	1.42×10^7
c_n	1.0	1.0	1.0
c_p	1.0	1.0	1.0

[†] after Selberherr [28]

[‡] after Raghunathan [29]

for $A_{n,p}$, $B_{n,p}$, and $c_{n,p}$ were obtained via extrapolation of coefficient parameters from silicon [28] and silicon carbide [29] based on the bandgap of diamond. These parameters are listed in Table IV.

IV. RESULTS AND DISCUSSION

The device structure in Fig. 1 was numerically simulated utilizing the models for intrinsic layer approximation, incomplete ionization of dopants, and unified concentration- and

Fig. 7. Numerically extracted hole and boron concentrations, and hole mobility through a Au-diamond Schottky m-i-p⁺ diode with $L_I = 10 \mu\text{m}$, taken at $V_A = 0 \text{ V}$, indicating the successful implementation of the mobility and activation models reflecting physical phenomena in single-crystal diamond layers.

temperature-dependent hole mobility given earlier. The simulated device structure was, however, modified to have a $2\text{-}\mu\text{m}$ p⁺ bulk as opposed to the thick bulk layer ($300\text{--}500 \mu\text{m}$) used during actual device fabrication to prevent excessive node count (thus economizing on computational overhead during device simulation). While it has been shown [6] that the resistivity of p⁺ layers with $N_A = 2.0 \times 10^{19} \text{ cm}^{-3}$ is approximately $90 \Omega \cdot \text{cm}$ at 300 K, the fabrication of the layered i-p⁺ stack of the Schottky m-i-p⁺ diode results in the formation of defects within the p⁺ layer, thus resulting in a sizeable substrate resistance R_{sub} in some of the fabricated devices. R_{sub} is thus a device- and process-dependent component and has been included as a series resistance to the numerical device structure, as shown in Fig. 1, and simulates the physical effect of the $300\text{--}500\text{-}\mu\text{m}$ synthetic diamond substrate. Fig. 7 shows the carrier (hole) concentration and mobility across a vertical cross section through a diamond-Au Schottky m-i-p⁺ diode with $L_I = 10 \mu\text{m}$ at zero bias predicted by the models. The effect of ϕ_{BP} on the drift carrier concentration justifies the use of $N_A(i') = 10^{11} \text{ cm}^{-3}$, where the drift layer is completely depleted by the Schottky anode as $p < N_A(i')$ for $y < 10 \mu\text{m}$, as would be the case for a completely intrinsic drift layer. In addition, $\mu_p(i) = 3800 \text{ cm}^2/\text{V} \cdot \text{s}$ while $\mu_p(p^+) \sim 55 \text{ cm}^2/\text{V} \cdot \text{s}$, which agrees with data obtained from material characterization [2], [6], [14].

A. Forward Conduction

Experimentally obtained forward characteristics of Schottky m-i-p⁺ single-crystal diamond diodes (fabricated to have the structure shown in Fig. 1 with Al and Au Schottky cathode contacts) are graphically shown in Fig. 8 for diodes with $L_I = 10\text{--}16 \mu\text{m}$. Also shown in the figure are the numerically obtained current-voltage (I - V) curves of devices with similar structure utilizing the models derived in this paper. Numerical

Fig. 8. Experimental forward characteristics of diamond Schottky m-i-p⁺ diodes with Au and Al cathode contacts and $L_I = 10\text{--}16 \mu\text{m}$, measured at 300 K. Numerically obtained results with the models derived in this paper are also shown in the figure.

analyses of devices are usually expected to give overoptimistic interpretations of the current capability of devices due to the inability to model physical phenomena such as defects, traps, and dislocations in the material. However, from the plots, it is evident that at 300 K, very good correlation between experimental and numerical forward characteristics is achieved with an error of 7%–11% in the voltage range $V_{\text{TO}} < V < V_{\text{TO}} + 2 \text{ V}$, over which a practical Schottky diode would be expected to operate.

At zero bias, the depletion region resulting from the potential barrier posed by the Schottky electrode extends into the drift region of the diode. As such, the current conduction mechanism

Fig. 9. Calibration of the Mott-Gurney law in (10) to the forward characteristics of a 3- μm Al Schottky m-i-p⁺ diode at 300 K gives $m_2 = 2.63$ for $n_1 = 2$.

in these Schottky m-i-p⁺ diodes is essentially SCL [9], where the hole concentration in the intrinsic drift layer, injected from the p⁺ bulk layer when forward biased $p_{\text{inj}}(\text{p}^+)$, is well in excess of the background carrier concentration in the drift region n_i , i.e., $p_{\text{inj}}(\text{p}^+) \gg n_i$. This results in the superlinear forward characteristics observed in Fig. 8 which is classically described by the Mott-Gurney relation [30] for SCL current

$$J = \frac{9}{8} \varepsilon_r \varepsilon_0 \mu_p \frac{V_A^{n_1}}{L_I^{m_2}} \quad (10)$$

where J is the current density through the material, ε_r and ε_0 are the relative and absolute permittivities, respectively, μ_p is the (concentration dependent or unified) hole mobility, $n_1 = 2$, and $m_2 = 3$. However, (10) does not account for carrier diffusion from the p⁺ bulk, ohmic losses due to imperfections in the contacts, and electrically active defects within the diamond crystal structure that affect current conduction through the device. Fig. 9 shows the I - V characteristics obtained experimentally for an Al Schottky m-i-p⁺ diode with $L_I = 3 \mu\text{m}$ and calculated curves based on (10) for $n_1 = 2$ with m_2 as a parameter. From the calibration curves, we obtain $m_2 = 2.63$ ($n_1 = 1.38$ from similar treatment), although these are dependent on the intrinsic length L_I which should not be the case for a pure intrinsic crystal. The results of this analysis indicate that current transport through the diamond Schottky m-i-p⁺ diode is complex and does not comprise solely of SCL current.

With respect to the results shown in Fig. 8, a distributed series R_{sub} component ranging between 15 and 70 $\text{m}\Omega \cdot \text{cm}^2$ was included in the numerical simulations to account for the varying substrate qualities and thicknesses of diodes 1–4. The lack of superlinearity in the I - V characteristics of diode 3 is due to the effect of the thicker intrinsic layer used for the drift region in this device. Numerical investigation of devices with 16- μm -thick drift layers reveals that the intrinsic layer is not completely depleted by the Schottky cathode at zero bias,

Fig. 10. Experimentally and numerically obtained temperature variation of forward characteristics for 10- μm Au Schottky m-i-p⁺ diodes for the temperature range of $T < 600$ K.

thus accounting for the additional resistive series component (attributed to the undepleted region of the “lowly doped” drift layer) to the overall current conduction mechanism through the diode. This accounts for the resistive linear characteristics seen for diode 3 for $V_A > 5$ V. It must be noted that Φ_M of the cathode electrode has been adjusted such that the numerically calculated V_{TO} matches that obtained experimentally due to the inability to model the traps and surface states and their influence on the surface potential barrier ϕ_{BP} . The experimental V_{TO} ’s obtained for the Al and Au–diamond Schottky m-i-p⁺ diodes were 1.0 and 2.0 V, respectively, at 300 K [31], [32].

The temperature sensitivity of the forward characteristics of Au Schottky m-i-p⁺ diodes is demonstrated both numerically and experimentally in Fig. 10. The unified hole mobility model $\mu_p(N_A, T)$ described in (7) and (8) has resulted in numerical characteristics that give excellent agreement with experimental results, within 2%–8%, for $T < 600$ K, giving a current density of 7.45 A/cm^2 for $V_A - V_{\text{TO}} = 3.3$ V at 507 K. The close correlation seen between numerical and experimental characteristics also indicates the suitability of the models derived in accounting for the temperature dependence of carrier transport in single-crystal CVD diamond.

B. Reverse Blocking Capability

Au–diamond Schottky m-i-p⁺ diodes (with $L_I = 18 \mu\text{m}$) were biased into reverse conduction in order to investigate the blocking capability of these devices. The characteristics of two such diodes are shown in Fig. 11, indicating breakdown voltages V_{BR} ’s in excess of -1.2 kV. The increase in leakage current observed can be attributed to the lack of termination structures on the physical device, as well the influence of point defects, dislocations, and stacking faults on the reverse performance of these diodes. Point-contact measurements on the same sample using a spring-loaded gold probe setup shown in the inset of Fig. 11 gave V_{BR} values in the range of -950 V to -1.7 kV. This voltage spread is indicative of surface

Fig. 11. I - V curves obtained from biasing 18- μm Au Schottky m - i - p^+ diodes into a reverse blocking mode, using gold push-down electrodes. Breakdown voltages obtained on these two samples were in excess of 1.2 kV.

Fig. 12. (a) Luminescence images of the top surface of a layered 5-mm square i - p^+ diamond sample as grown ($L_I = 20 \mu\text{m}$). (b) Array of Au Schottky dots fabricated on the sample (radii indicated in the image).

inhomogeneity that results during the growth of the layered i - p^+ diamond stack structure.

The areal defect distribution on a 20- μm i - p^+ stacked diamond layers is presented in the optical luminescence images of Fig. 12(a). The bright spots on the sample are due to defects that terminate at the surface (the best areal defect densities are in the range 10^3 – 10^4 cm^{-2}). Circular Au Schottky contacts fabricated on this layered diamond structure are shown in Fig. 12(b). Unpatterned ohmic contacts have been fabricated on the backside of the sample. These diodes were reverse biased, and the breakdown voltage variation obtained across a 2.7-mm square area on the sample is shown in Fig. 13 for Au Schottky contacts of diameters 200 and 50 μm . Diodes that were able to withstand reverse anode voltages in excess of 1.1 kV are located

interior to the sample. From the contour plots, it is evident that diodes with smaller fabricated contacts are able to exceed the nominal maximum reverse voltage of 1.1 kV without going into avalanche. This indicates a decreased susceptibility of the breakdown voltage to defective material in the diamond i - p^+ layered stack due to the reduced likelihood of trap and defect inclusion under smaller contacts.

Calculations utilizing the impact ionization model in (9) and the extrapolated ionization coefficient parameters listed in Table IV gave a numerical V_{BR} of -2.27 kV for an un-terminated Au–diamond Schottky m - i - p^+ diode with leakage currents on the order of 10^{-27} A/cm^2 , for $L_I = 18 \mu\text{m}$. This is 25% higher than the best blocking voltage demonstrated experimentally. This numerically predicted V_{BR} is an approximate

Fig. 13. Breakdown voltage contour maps highlighting variation across a 2.7-mm square array on the same sample. V_{BR} 's obtained from (a) 200- μm - and (b) 50- μm -diameter circular Schottky anode contacts are shown (similar legends are used for both maps).

gauge of the blocking capability of diamond devices, as the parameters implemented in (9) were assumed to scale with bandgap, which may not actually be the case. It is noteworthy that the peak electric field obtained numerically was 1.88 MV/cm, a value that is significantly lower than the 20-MV/cm value that is the quoted standard for intrinsic diamond (see Table I). This is due to the quasi-intrinsic layer used in the simulator as opposed to a completely intrinsic layer. However, it is speculated that the lack of termination structure, rather than the quasi-i-layer doping, limits the ultimate breakdown capability of the device. Detailed studies pertaining to ionization integral coefficient parameters following the work of Raghunathan and Baliga [29] are currently underway [27] to obtain accurate impact ionization coefficient parameters for single-crystal CVD boron-doped diamond layers to enable accurate prediction of the reverse breakdown of diamond high-voltage devices.

V. CONCLUSION

We have successfully described intrinsic and boron-doped single-crystal CVD diamond for numerical device simulation. The models proposed are consistent with recent results obtained through material characterization. These models account for deep acceptors in diamond and hence address the different conduction regimes in the material attributed to the varying degrees of incomplete ionization of boron dopant. In addition, the unconventional use of completely intrinsic diamond layers in Schottky diode design was successfully modeled through simulation with numerical approximation of carrier-free material and a formulation of doping- and temperature-dependent (unified) carrier transport. The unified mobility model also accounts for high hole mobility measured in intrinsic CVD diamond. The accuracy of these models have been verified by the very good correlation observed between the numerically and experi-

mentally obtained forward characteristics of diamond Schottky m-i-p⁺ diodes in the 300–600-K temperature range. Due to the lack of data pertaining to impact ionization of carriers in reverse-biased i-p⁺ junctions in diamond, numerical analysis of the breakdown capabilities of these devices is approximate. In addition, at the current stage of diamond technology, the voltage handling capability of devices is limited by residual defects in the intrinsic voltage blocking layer in the device structure.

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