

Insights provided by TCAD modelling into on- and off-state performance of pseudo-vertical diamond Schottky barrier diodes[☆]

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ABSTRACT

Pseudo-vertical Schottky barrier diodes were fabricated on boron-doped diamond layers grown by microwave plasma chemical vapor deposition on high-pressure high-temperature and chemical vapor deposition substrates. Analysis of these devices by means of a coupled experimental/simulation approach has allowed on- and off-state operational regimes to be linked to technology-specific parameters, with the aim of providing useful indications for viable optimization routes. Specifically, compensation of boron doping by unintentional donor impurities like nitrogen is suggested to limit the diode on-state conductance, while acceptor surface defects are suggested to critically influence the reverse leakage current and breakdown, so that their reduction or passivation can enable significant breakdown voltage increase.

1. Introduction

Schottky barrier diodes (SBDs) are being intensively studied, as they might be the earliest, commercial diamond power devices. Vertical SBDs [1–5] have the potential for both high-current and high-voltage capabilities, besides allowing full exploitation of diamond thermal conductivity. However, they require costly, conductive diamond substrates. Lateral SBDs [6,7] use thin diamond layers on lower cost, insulating substrates, but are penalized by a stringent performance trade-off, as the long lateral spacing necessary for high breakdown voltages results in increased series resistance and small on-state current. Pseudo-vertical SBDs [8–12] represent a balanced cost-performance approach, combining lateral layout (therefore not requiring conductive substrates as in vertical SBDs) with vertical current flow (thus allowing a more relaxed trade-off between current capability and blocking voltage than lateral SBDs).

In this work, we report on experimental and Technology Computer Aided Design (TCAD) simulation results from two generations of

pseudo-vertical, diamond SBDs. The two generations differ for different growth time, substrate, and doping, with second generation aiming to reach better crystal quality in the active layer. The adopted, coupled experimental-simulation approach is aimed at gaining insight into the improvements achieved in both on- and off-state behavior from first to second generation and obtaining indications in view of further technology optimization.

2. Samples, experimental setup and numerical model

1st (SBD-1) and 2nd (SBD-2) generation of pseudo-vertical SBDs have been fabricated by DIAMFAB on boron-doped diamond layers grown by microwave plasma chemical vapor deposition (MPCVD). 1b high-pressure high-temperature (HPHT) substrates from Sumitomo have been used for SBD-1 fabrication run, whereas 11a chemical vapor deposition (CVD) substrates from EDP have been adopted for SBD-2. The change in the substrate type from 1st to 2nd generation was aimed at improving the crystal quality of grown diamond layers and

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benchmarking established HPHT substrates against cost effective CVD ones which is necessary for industrial scaling in the near future. Resulting diode cross sections are sketched in Fig. 1(a) and (b).

The device stack consists of a 0.5 μm heavily boron-doped layer grown on either HPHT or CVD substrates, with a boron concentration exceeding $3 \times 10^{20} \text{ at}/\text{cm}^3$, above the metal-insulator transition threshold. This layer is capped with a 2.86 μm or 2.0 μm , lightly boron-doped drift layer for the HPHT and CVD case, respectively. Targeted boron concentrations are $3 \times 10^{16} \text{ cm}^{-3}$ and $5 \times 10^{15} \text{ cm}^{-3}$ for SBD-1 and SBD-2 diodes, respectively. Reducing the boron concentration and thickness of the drift layer in SBD-2 diodes compared to SBD-1 ones was intentional and aimed at obtaining improved crystal quality of the drift layer and therefore improved electrical characteristics of the diodes. Reactive ion etching was used to access the buried heavily doped layer. Titanium ohmic contacts were then deposited on the heavily doped layer and subsequently annealed at 600 $^{\circ}\text{C}$ to promote TiC formation and reduce the contact resistance. The full ohmic stack is composed of a Ti/Pt/Au trilayer. Finally, molybdenum (Mo) Schottky contacts were deposited on the lightly doped layer following an ozone treatment to achieve oxygen surface termination, thereby increasing the Schottky barrier height. As reported by the microscopic images of individual mesas from the SBD-1 and SBD-2 generations, presented in the bottom row of Fig. 1, the surface quality improved in the second generation due to the reduction in crystallite density, suggesting a higher quality Schottky contact. The full Schottky contact stack is composed of a Mo/Pt/Au trilayer. No oxide passivation was implemented.

Diodes were tested by means of a parameter analyzer Keysight B1505 equipped so that it can measure medium- and high-voltage current versus voltage characteristics (I-V) and capacitance versus voltage (C-V) characteristics. Regarding I-V measurements, to reduce the instrument noise level below 10 pA, the ramped condition was chosen. The integration time was chosen to have high resolution and minimize possible self-heating. In addition, because the dominant heat dissipation pathway was between the substrate and the thermal chuck, whose thermal resistance is estimated to be approximately 10 K/W, the power dissipated by the diodes led to a negligible temperature increase relative to the temperature imposed by the thermal chuck. For the extraction of the Schottky barrier height (Φ_B), diodes were initially tested for temperature-dependent I-V characteristic that were then fitted by Shockley diode equation to extract the saturation current density, for each temperature, taking in account the effect of the series resistance. Φ_B

was then determined from the Richardson-Dushman equation by means of the Richardson's plot. This method was preferred over determining the built-in potential from the $1/C^2$ -voltage characteristics, because a reliable value could be extracted only for the SBD-1 generation. Specifically, within the investigated voltage range, the SBD-1 generation exhibited an almost linear $1/C^2$ -voltage dependence. In contrast, this behavior was not observed for the SBD-2 generation, for which a reliable value of the built-in potential could not be extracted. To extract the ideality factor, Shockley equation was rearranged and then the minimum as a function of the test voltage was selected.

C-V characteristics were then extracted for both diodes at $T = 300 \text{ K}$ in the voltage range from 0 V to 20 V, in reverse bias, at a frequency of 1 MHz with a small-signal amplitude equal to 50 mV. In the case of SBD-2, due to the low boron concentration, the depletion region at the maximum bias voltage almost reached the highly boron doped region.

For the high-voltage reverse-bias I-V characterization, devices were tested by repeated I-V characteristic up to the reaching of the current compliance at each iteration, followed by a forward-bias sweep to evaluate the appearance of shunts.

Two-dimensional numerical devices simulations have been carried out with the Sentaurus Device™ tool that is part of the Synopsys TCAD suite [13]. The adopted charge-transport model more specifically consists of the Poisson's equation, relating the electric-potential distribution with the total space-charge density, and the two carrier-continuity equations, in which the current densities for electrons and holes are expressed as the sum of the drift and diffusion contributions. All simulations shown in the following are, specifically, obtained by quasi-stationary voltage sweeps. Material-related models and their parameters have been set to values reported in the literature. These include: bandgap [14] and electron affinity [15], incomplete dopant ionization for boron [14] and nitrogen [16], temperature dependent mobilities [14], doping dependent mobilities [14], impact ionization [17]. As far as the incomplete ionization is concerned, it has to be noted that a static approximation has been assumed, whereas a more comprehensive description of its effects would require a fully dynamic, trap model to be used for the dopant levels, in conjunction with transient simulations [18,19]. Dynamic effects related to fast voltage sweeps are therefore not captured by our simulations. At the Schottky contact, hole tunneling injection has been accounted for, in addition to thermionic emission, by activating the simulator's non-local tunneling model based on the WKB approximation [13]. Deep levels are modelled within the simulator by means of the Shockley-Read-Hall (SRH) detailed balance equation relating the level occupancy to the microscopic electron and hole emission and capture processes. The mathematical model has been solved in cylindrical coordinates, which, for the simulated, circular-symmetry diodes, is equivalent to carrying out 3D simulations. Simulated diodes have specifically a diameter of the Schottky contact equal to 140 μm and 100 μm for the SBD-1 and SBD-2 case, respectively. TCAD modelling of diamond SBDs has already proved to be a useful tool to complement experimental analysis and provide interpretation for several, key features of these under-development devices [14–24].

3. Experimental results

Main electrical parameters extracted from the characterization of both fabrication runs are summarized in Table 1. As can be noted, a remarkable, 160-times increase in the room-temperature, on-state current density at $V = -10 \text{ V}$ is achieved in the SBD-2 diodes on CVD substrates, despite the reduced drift layer doping. Correspondingly, the specific on-state resistance ($R_{\text{ON}} \text{ A}$) improves from 3.7 $\Omega \text{ cm}^2$ to about $10 \times 10^{-3} \Omega \text{ cm}^2$. These on-state performance improvements come along with a 0.46 eV Schottky barrier increase, which denotes the achievement of a more ideal Schottky contact. On the other hand, SBD-2 diodes exhibit a slightly increased ideality factor. The extracted values of the ideality factor and Richardson's constant, that are consistent with those reported in the literature for non-annealed contacts [25–27],

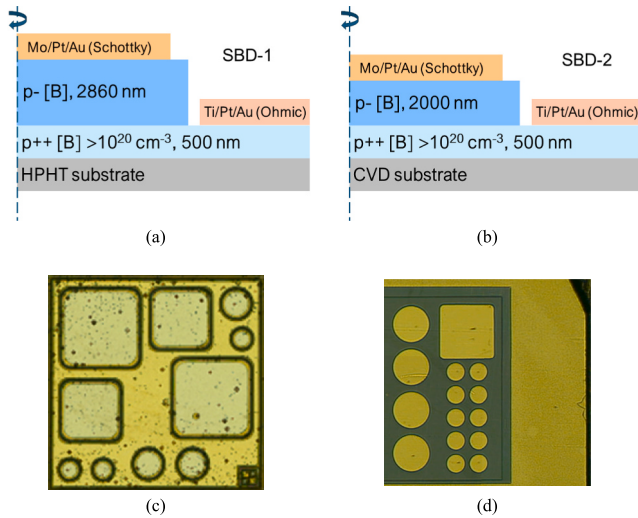


Fig. 1. In the top row: schematic cross section of SBD-1 (a) and SBD-2 (b) Schottky barrier diodes. Dashed lines indicate the rotational axis of the simulated, circular devices. In the bottom row: microscope images of a single mesa of tested devices, showing the diodes of different areas and shapes available on SBD-1 (c) and SBD-2 (d).

Table 1

Main electrical parameters of SBD-1 and SBD-2 diodes. Data ranges refer to measurements from 28 samples of different shapes (rectangular, circular) and area.

Generation	SBD-1	SBD-2
On-state current density @ -10 V and $T = 300$ K	$(2.9 \pm 0.4) \text{ A/cm}^2$	$(4.6 \pm 0.9) \times 10^2 \text{ A/cm}^2$
On-state current density @ -5 V and $T = 300$ K	$(1.5 \pm 0.2) \text{ A/cm}^2$	$(18 \pm 4) \text{ A/cm}^2$
Rectification ratio @ ± 10 V and $T = 300$ K	$> 2 \times 10^4$	$> 10^{10}$
Schottky barrier height, Φ_B	$(0.91 \pm 0.09) \text{ eV}$	$(1.37 \pm 0.02) \text{ eV}$
Ideality factor	1.7 ± 0.2	1.8 ± 0.1
Specific on-state resistance, $R_{ON} \cdot A$	$(3.7 \pm 0.7) \Omega \text{ cm}^2$	$(10 \pm 7) \times 10^{-3} \Omega \text{ cm}^2$
Reverse voltage @ 10^{-5} A/cm^2 and $T = 300$ K	$(16 \pm 8) \text{ V}$	$(1.6 \pm 0.5) \times 10^2 \text{ V}$
Breakdown voltage (device failure)	115 V	430 V

indicate that there is still scope for improving the quality of the Schottky contacts. Improvements can also be noticed on the rectification factor at ± 10 V, showing an increase of more than 5 orders of magnitude, where, in the case of SBD-2 diodes, the reverse current at 10 V is dominated by the noise level of the instrument.

Fig. 2(a) and (b) shows the measured C-V characteristics at $T = 300$ K from different SBD-1 and SBD-2 diodes. The curves show consistency in each generation taking into account intra-wafer variability of the samples. In addition, the impedance phase measured stayed always around -90° suggesting the quality of the measurement. From those measurements, the experimental effective doping concentration ($N_A - N_D$) profiles are extracted and shown in Fig. 2(c) and (d). The nominal boron doping

values are included as dashed lines. As can be seen, the effective doping is smaller than the nominal doping for both SBD-1 and SBD-2 diodes, indicating that boron doping is partially inactive and/or compensated by unintentional donor impurities like nitrogen. It is worth noticing that the measurement frequency was not affecting the extraction of the effective doping profile in the range of interest showing no dependence with frequency smaller to 1 MHz. The ($N_A - N_D$) values adopted in the simulations and plotted in Fig. 2 as dotted lines will be commented in Section 4.

Fig. 3 shows experimental, forward-bias current-density (J) vs voltage (V) curves at different temperatures (T) for representative diodes from SBD-1 and SBD-2 generations. Simulation results, included in Fig. 3, will be commented in Section 4. As can be noted, the SBD-2 diode is characterized, in the high forward-bias regime, by a steeper slope of the J-V curve. More precisely, one finds that the $\log(J)$ - $\log(V)$ curve approaches a line with slope equal to 1 and 2 for the SBD-1 and SBD-2 case, respectively (not shown for brevity). This indicates that, for the SBD-2 diode, high-current conduction is impacted by space-charge effects in the p-, drift layer, so that on-state current is due to space-charge-limited current (SCLC) rather than ohmic current [28,29]. The latter is instead the limiting conduction mechanism for SBD-1 diodes at high forward bias.

As far as the off-state behavior is concerned, SBD-1 diodes are characterized by a reverse voltage at $J = 10^{-5} \text{ A/cm}^2$ of $(18 \pm 4) \text{ V}$ at $T = 300$ K. Biasing the diodes at more than 100 V induces a significant degradation in the electrical behavior of the devices, which is put into evidence by repeated I-V characterization showing a $\times 10^4$ increase in the low-voltage, reverse current after a first voltage sweep up to 115 V. This is illustrated by Fig. 4 for a representative SBD-1 diode. The increase in reverse leakage current observed after the first sweep in this

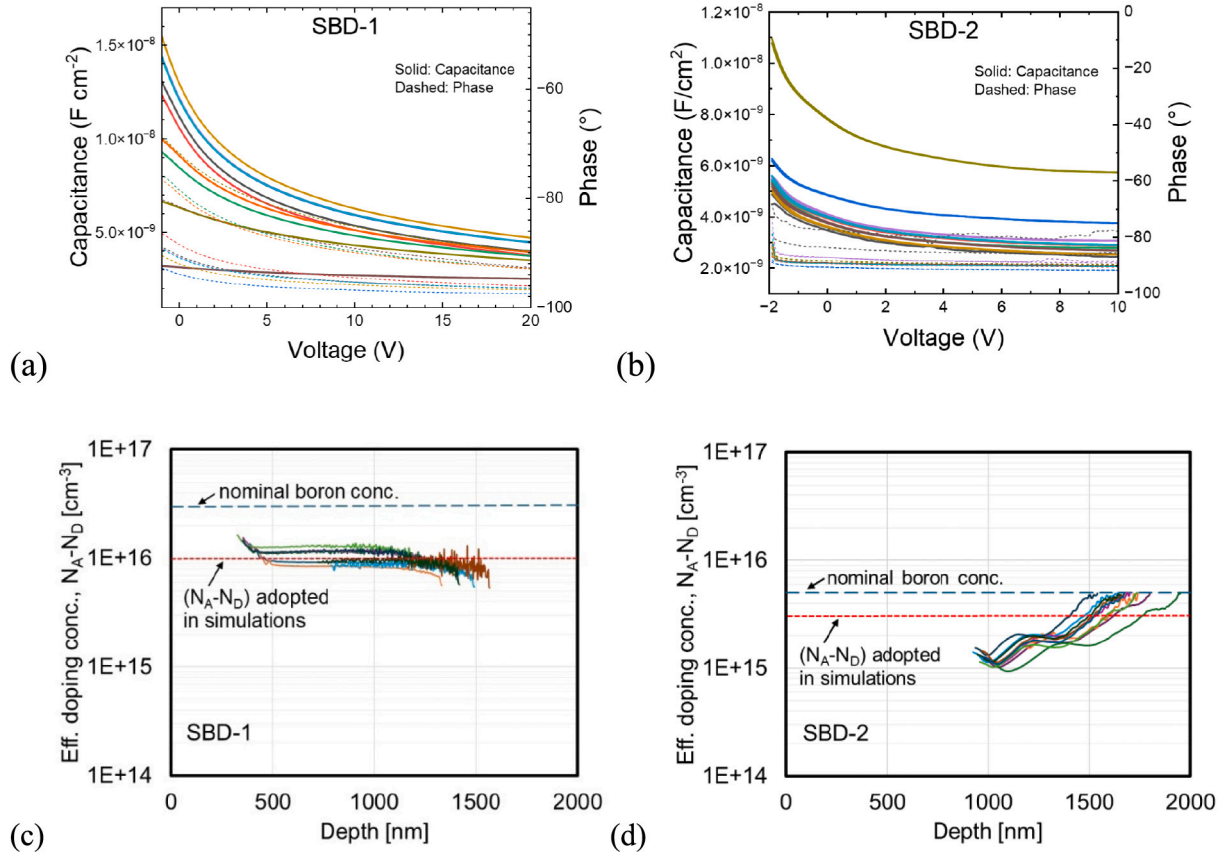


Fig. 2. In the upper row, C-V characteristics at $T = 300$ K for SBD-1 (a) and SBD-2 (b) generations. Capacitance is in solid lines, and the impedance phase is in dashed lines. In the lower row, extracted experimental effective doping concentration ($N_A - N_D$) versus depth for SBD-1 (c) and SBD-2 (d) diodes. The blue dashed lines denote the nominal boron concentration values. The red dotted lines are the ($N_A - N_D$) values adopted in the simulations.

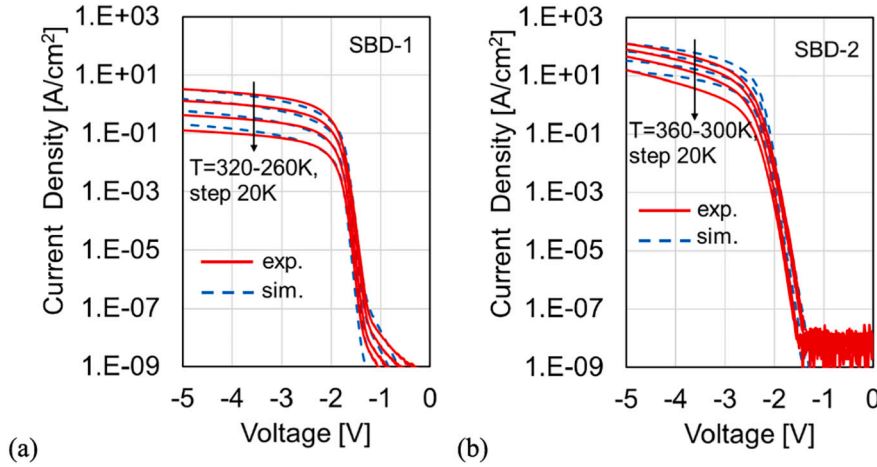


Fig. 3. Experimental and simulated, forward-bias current-density vs voltage curves at different temperatures for a representative diode from the SBD-1 (a) and the SBD-2 (b) generation. Both diodes have circular symmetry with a diameter of 140 μm and 100 μm for the SBD-1 and SBD-2 case, respectively.

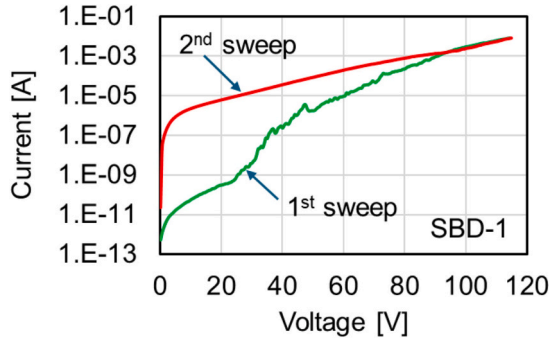


Fig. 4. Repeated, experimental reverse-bias current-density vs voltage curves of a representative diode from the SBD-1 generation at $T = 300$ K. The diode has circular symmetry with 140- μm diameter.

generation is indicative of percolative conduction paths that become electrically active. The origin of these percolative paths can be ascribed to dislocations in the vertical p-layer. The presence of these dislocations can be inferred from the optical image in Fig. 1(c). This should be compared with the lower defect density exhibited by the second generation, as shown in Fig. 1(d).

SBD-2 diodes are characterized by a reverse voltage at $J = 10^{-5}$ A/ cm^2 of $(1.6 \pm 0.5) \times 10^2$ V at $T = 300$ K and by a maximum applicable voltage of 430 V before device failure, with a remarkable improvement

over SBD-1 devices. I-V characterization under repeated reverse voltage sweeps is illustrated by Fig. 5 for a representative SBD-2 diode. No appreciable change in the I-V curves is observed under repeated reverse-bias sweeps if these are limited to a maximum reverse bias of 400 V. Curve #1 is representative of such repeatable I-V curves. Device failure occurs at about 430 V as shown by curve #2. Curve #3 is finally representative of a failed diode. Some of the tested SBD-2 diodes showed burned point on the edge of the Schottky contact, corresponding to the failure point, as can be seen in Fig. 5 (b). Such an improvement in the high reverse bias behavior of SBD-2 devices compared to SBD-1 ones, can tentatively be attributed to an improvement in the diamond crystal quality, including at the device surface where the electric field is expected to peak. Simulations shown in Section 4 will provide additional insight into this possibility.

4. Simulation results

TCAD simulations have been adopted to gain insight into performance improvements shown by SBD-2 diodes compared to SBD-1 ones.

On-state performance is influenced by several parameters, including the active boron doping within the drift-layer, the concentration of possible donor impurities like nitrogen, as well as hole mobility. TCAD simulations can help disentangling the effects of these parameters. To this purpose, Fig. 6 shows forward-bias, experimental J-V curves for representative SBD-1 and SBD-2 diodes at the same temperature (320K). The experimental data are compared to simulations assuming: (i) nominal boron concentrations with no deep donor compensation and

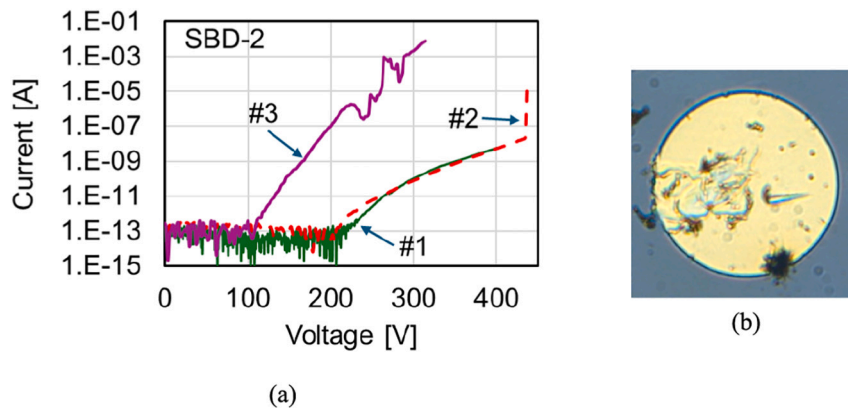


Fig. 5. (a) Repeated, experimental reverse-bias current-density vs voltage curves of a representative diode from the SBD-2 generation at $T = 300$ K. The diode has circular symmetry with 100- μm diameter. (b) Representative failed diode from SBD-2 generation that shows a burned point on the edge of the Schottky contact.

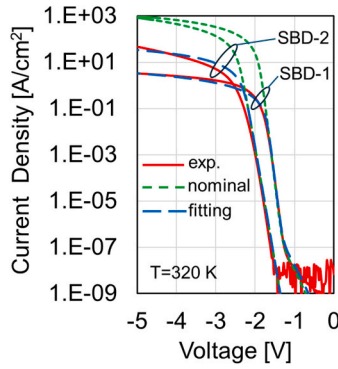


Fig. 6. Experimental J-V curves at 320 K for representative diodes from the SBD-1 and SBD-2 generations (red solid lines), compared to simulations assuming: (i) nominal boron concentrations with no deep donor compensation and unmodified hole mobility (green dotted lines) and (ii) compensating donors and, for SBD-1, modified maximum hole mobility (blue dashed lines), as required to fit measurements.

the hole mobility model reported in [14] with unmodified parameters, and (ii) nominal boron doping partially compensated by suitable densities of deep donors. In the case of the SBD-1 diode only, also a modified maximum hole mobility is taken in account for (ii). According to simulations, the thickness of the p++ layer has a negligible influence on J_{ON} and (R_{ON} A) provided it is made greater than 250 nm.

First of all, to fit the thermionic-emission regime, the Mo work function (WF) had to be set to 5.0 eV for the SBD-1 diode. On the other hand, a WF of 4.4 eV is required for fitting the SBD-2 diode J-V curve. Both WF values are within the reported range for Mo [30–32] and the WF change of 0.6 eV is comparable with the measured Φ_B increase of 0.46 eV from SBD-1 to SBD-2. Besides thermionic emission, hole tunneling injection has been activated at the Schottky contact. To reproduce the J-V slope in low forward-bias regime, the hole tunneling mass had to be set to 0.6 and 0.5 for the SBD-1 and SBD-2 diode, respectively, consistently with the larger ideality factor of the 2nd diode generation.

In the high-current regime, the on-state current density appears to be limited by the high resistivity of the drift layer, due to light boron doping and possible compensation effects by deep donors, further reducing the effective p-type doping. Concerning the resulting conduction mechanism, as already observed in Section 3, J_{ON} is dominated by ohmic current and SCLC for the SBD-1 and SBD-2 case, respectively. In this respect, it has to be considered that simulations solve the drift-diffusion equations for current densities self-consistently with the Poisson's equation, so they are able to describe space-charge effects and related SCLC more accurately than analytical models. In the simulations, the boron concentration in the drift layer was set to the nominal, targeted values of 3×10^{16} and $5 \times 10^{15} \text{ cm}^{-3}$ for the SBD-1 and SBD-2 diode, respectively. As can be noted in Fig. 6, if no donor compensation is assumed, the SBD-2 diode would have a slightly smaller J_{ON} compared to the SBD-1 one, as reported by the “nominal” curves (i) plotted as green dotted lines in Fig. 6. This results from the lower boron concentration in the drift layer, that is only partially compensated by the reduced thickness. On the other hand, actual SBD-2 diodes are characterized by a factor of ≈ 12 increase in J_{ON} at $V = -5$ V. To comply with measurements of the effective doping concentration shown in Fig. 2, unintentional deep donors were added within the drift layer. These were assumed at an energy of 1.7 eV from the conduction band, corresponding to nitrogen impurities. For simplicity, uniform profiles have been adopted for both boron and nitrogen. Nitrogen concentration was specifically set to 2×10^{16} and $2 \times 10^{15} \text{ cm}^{-3}$, so that the effective ($N_A - N_D$) doping is 1×10^{16} and $3 \times 10^{15} \text{ cm}^{-3}$, for the SBD-1 and SBD-2 diode, respectively. These values are included as dotted lines in Fig. 2. Notably, including the above values of nitrogen concentration is

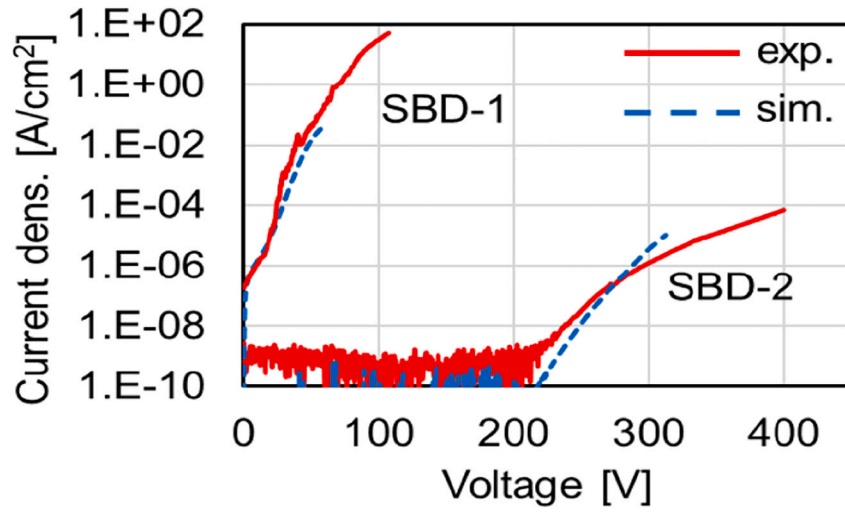
sufficient to obtain a simulated J-V curve in reasonable agreement with the experiments for the SBD-2 diode, without having to assume any degradation of the maximum, room-temperature hole mobility (corresponding to the undoped diamond limit) from its literature value of $2016 \text{ cm}^2/(\text{V s})$ [14]. For the SBD-1 diode, a degradation of the maximum, room-temperature hole mobility to $1100 \text{ cm}^2/(\text{V s})$ had, instead, to be assumed in the simulations, in addition to boron compensation, to fit measurements. The outcomes of this fitting procedure are reported in Fig. 6 as “fitting” curves (ii) plotted as blue dashed lines. Adopted boron and nitrogen concentrations are to be intended as average values, since effective doping concentration resulting from measurements in Fig. 2 are actually non uniform. This can lead to inaccuracies in the (i) compensation ratio estimate and (ii) depletion-region width and electric-field profile calculation. Moreover, since a fraction of the introduced boron can be inactive, the adopted nitrogen concentration must be considered as possibly overestimated, “effective” values, accounting for the total difference between nominal boron concentration and effective doping.

Simulated, forward-bias J-V-T curves obtained with the same parameters adopted for fitting curves in Fig. 6, have been included in Fig. 3 (a) and (b). As can be noted, an overall satisfactory agreement between experiments and simulations is maintained also at varying temperatures.

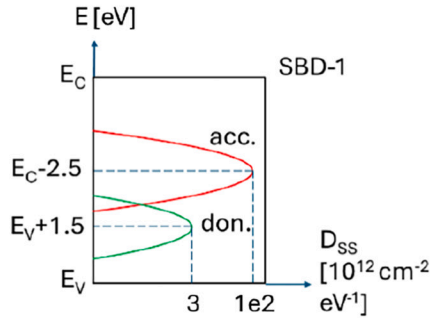
Turning now our attention to the off-state regime and specifically focusing on the room-temperature, high reverse-voltage regime, general insights provided by TCAD simulations are as follows: (i) reverse leakage current in the pre-breakdown regime can be explained by hole tunneling injection from the Schottky contact, whereas impact ionization comes into play at higher voltages, as the electric field approaches the critical field for avalanche; (ii) the reverse current level is critically dependent on the electric-field peak at the Schottky-metal corner onto the exposed diamond surface; (iii) the surface trap density distribution has a critical impact on the electric-field peak; (iv) donor-like traps help extending laterally the Schottky junction depletion region, mitigating the electric-field peak and thus reducing the reverse leakage current and shifting the breakdown voltage to larger values; (v) on the other hand, acceptor-like traps pinches the depletion region at the metal corner, enhancing the electric-field peak and thus reducing the breakdown voltage.

To model the diamond surface, we assumed a density of surface states (D_{SS}) dominated by amphoteric dangling bonds, resulting in both acceptor-like and donor-like traps, with the donor traps closer to valence band than the acceptor ones [33]. Gaussian energy distributions with 1-eV standard deviation were assumed for both acceptor and donor traps. These traps were placed throughout the top, unmetallized surface of the p⁺ diamond layer. By using this basic model, a reasonable agreement between simulated and experimental high-voltage, reverse-bias J-V curves has been pursued, by adjusting the peaks and energy positions of the assumed acceptor- and donor-trap distributions. In the absence of detailed experimental results on D_{SS} , the adopted approach must be intended as a proof-of-concept for the hypothesis that the strikingly different reverse breakdown behavior characterizing the two diode generations can be correlated, in these devices with no termination structures, simply to a different D_{SS} at the exposed diamond surface.

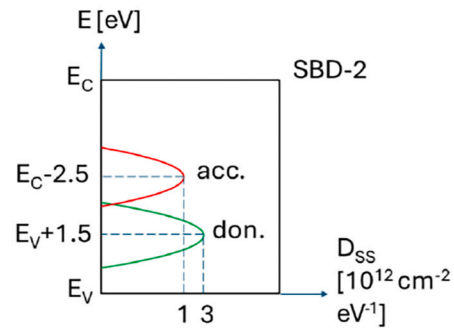
The outcome of this analysis is illustrated by Fig. 7(a), showing simulations of the reverse-bias current density, compared to measurements already shown in Figs. 4 and 5 (1st-sweep curves only) for a SBD-1 and SBD-2 diode, respectively. In the case of the SBD-1 diode, D_{SS} peaks of 1×10^{14} and $3 \times 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$ are assumed for acceptors and donors, respectively. In the case of the SBD-2 diode, D_{SS} peak values are 1×10^{12} and $3 \times 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$. Peak energies of the two Gaussian distributions are the same for SBD-1 and SBD-2 simulations, namely 2.5 eV from the conduction-band edge for acceptors and 1.5 eV from the valence band for donor traps. A schematic illustration of the above D_{SS} distributions is shown in Fig. 7(b) and (c). As can be noted from Fig. 7(a), with the assumed D_{SS} pattern, simulations are able to qualitatively capture the strong reduction in the reverse-bias current of the SBD-2 diode compared to SBD-1 one, corroborating the possible link between



(a)



(b)



(c)

Fig. 7. (a) Experimental and simulated reverse-bias current density vs voltage curves of representative SBDs from the SBD-1 and SBD-2 fabrication runs. The two diodes have both circular symmetry with 140- μm and 100- μm diameter in the SBD-1 and SBD-2 case, respectively. Schematic D_{SS} adopted for the simulated (b) SBD-1 and (c) SBD-2 diodes.

high-voltage handling capability and surface charges. More precisely, the poor off-state performance of SBD-1 diodes may be linked to a large density of surface acceptors. Conversely, the improved performance of SBD-2 diodes can be explained by a reduction of these surface acceptors (a factor of 10^2 reduction in our simulations). For both diodes, simulations stopped converging before the onset of avalanche breakdown and hole tunneling from the Schottky contact remained the dominant reverse-bias current mechanism up to the last simulated point.

Fig. 8(a) and (b) shows 2D contour plots of the hole-density distribution within the simulated SBD-1 and SBD-2 diodes at the same reverse voltage of 50 V. As can be noted, the depletion region develops vertically beneath the Schottky contact in the SBD-1 device and a very high electric field develops at the metal corner due to the large equipotential lines curvature. This is actually what is expected for diodes without any dedicated termination structure, like those considered here. A high density of surface acceptor traps can only exacerbate this effect, as surface acceptors locally increase the negative space charge (acting like “additional p-type doping”). On the contrary, the depletion region extends also laterally under the uncontacted surface in the SBD-2 diode. This is the effect of the smaller, surface acceptor density assumed for the SBD-2 diodes, leaving surface donors as the dominant traps and allowing the associated positive charge to deplete the underneath diamond layer. This lateral propagation of the depletion layer relaxes the curvature of

the equipotential lines at the metal corner, thus reducing the electric-field peak thereby. Fig. 8(c) shows the electric field along a horizontal cutline at the device surface (see line h1 in plots (a) and (b)) for a reverse voltage close to the highest simulated value, namely 50 V and 300 V for the SBD-1 and SBD-2 diode, respectively. As can be noted, the electric field reaches the same peak value of $4\text{--}5 \times 10^6$ V/cm in both cases, but, in the SBD-2 diode, this takes place at a 6-times larger reverse voltage.

5. Conclusion

Two generations of pseudo-vertical diamond Schottky barrier diodes, respectively fabricated on HPHT and CVD diamond substrates, have been analyzed by TCAD simulations, with the aim of gaining insight into the improvements in both on- and off-state performance characterizing the 2nd generation compared to the 1st one.

These improvements include -in spite of the reduced, targeted boron doping concentration in the drift layer- in a $160\times$ increase in the on-state current density at a voltage of -10 V and a $12\times$ increase at -5 V. TCAD analysis suggests this on-state performance improvement can be related to a reduced boron doping compensation by deep donors in the lightly doped drift layer and a higher hole mobility.

2nd generation diodes exhibit also an improved off-state performance, with a maximum applicable reverse voltage before device failure

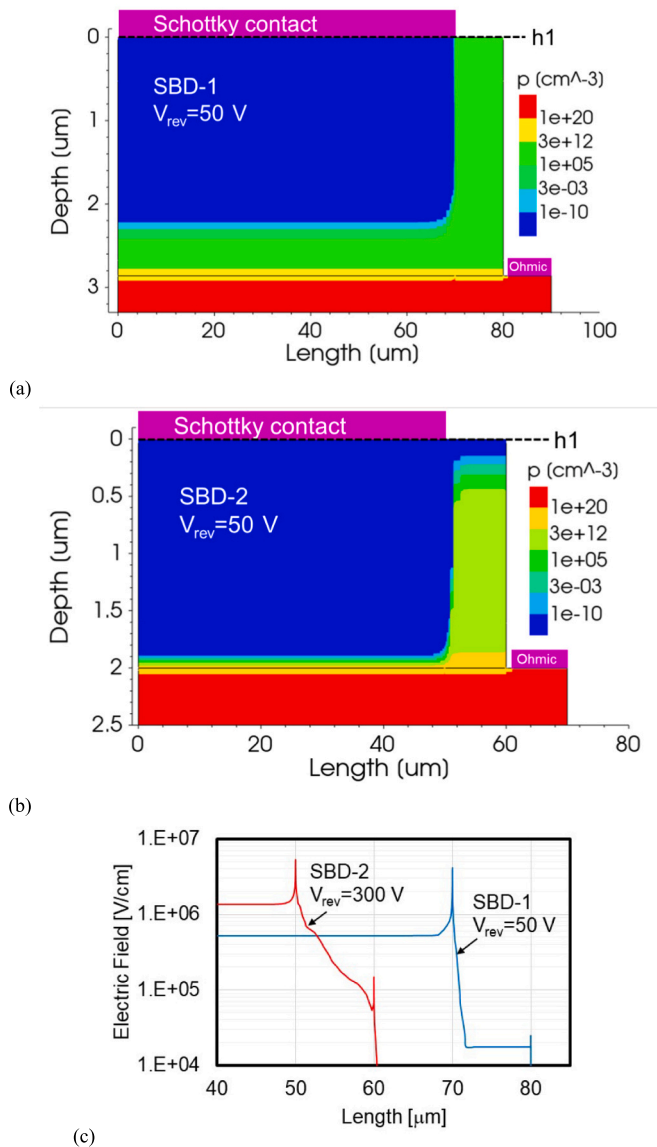


Fig. 8. 2D contour plots of the hole-density distribution within the simulated (a) SBD-1 and (b) SBD-2 diodes at a reverse voltage of 50 V. In (c) a 1D plot of the electric field along surface cutlines (h1 on a) and b)) is plotted for voltages close to the highest simulated reverse voltage, namely 50 V and 300 V for the SBD-1 and SBD-2 diode, respectively.

of 430 V (115 V for 1st generation) and a reverse voltage at $J = 10^{-5}$ A/cm² and 300 K of $(1.6 \pm 0.5) \times 10^2$ V ((16 ± 8) V for 1st generation). TCAD analysis suggests that the improved off-state performance may be related to a better diamond surface quality and specifically to a reduced surface acceptor trap density.

The development of a TCAD modelling framework, able to provide results in quantitative agreement with the performance of actual devices from two generations characterized by markedly different crystal quality and electrical performance, is important for understanding power devices for future device optimization and pushing diamond devices to their theoretical limits.

CRedit authorship contribution statement

Giovanni Verzellesi: Writing – review & editing, Writing – original draft, Supervision, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Giacomo Biasin:** Writing – review & editing, Methodology, Investigation, Data curation,

Conceptualization. **Julien Bassaler:** Writing – review & editing, Methodology, Investigation, Data curation, Conceptualization. **Matteo Bufolo:** Writing – review & editing, Methodology, Investigation, Conceptualization. **Vishwajeet Maurya:** Writing – review & editing, Methodology, Investigation, Data curation. **Alessandro Chini:** Writing – review & editing, Methodology, Investigation, Conceptualization. **Carlo De Santi:** Writing – review & editing, Methodology, Investigation, Data curation, Conceptualization. **Manuel Fregolent:** Writing – review & editing, Methodology, Investigation, Data curation. **Gaudenzio Meneghesso:** Supervision, Methodology, Investigation, Funding acquisition, Conceptualization. **Enrico Zanoni:** Supervision, Methodology, Investigation, Funding acquisition. **Juliette Letellier:** Writing – review & editing, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Matteo Meneghini:** Writing – review & editing, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare no conflict of interest.

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Data availability

The authors do not have permission to share data.

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