

Quantum-enhanced electric field mapping within semiconductor devices

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Semiconductor components based on silicon carbide (SiC) are a key component for high-power electronics. Their behavior is determined by the interplay of charges and electric fields, which is typically described by modeling and simulations that are calibrated by nonlocal electric properties. So far, the 3D mapping of both the electric field and the concentrations of free charge carriers inside an electronic device remains a challenging task. To fulfill this information gap, we propose an operando method that utilizes single silicon vacancy (V_{Si}) centers in 4H-SiC. The V_{Si} centers are at various positions in the intrinsic region of a p - i - n diode. To monitor the local static electric field, we perform Stark-shift measurements based on photoluminescence excitation, which allows us to infer the expansion of the depletion zone and therefore to determine the local concentration of dopants. Besides this, we show that our measurements allow us to additionally obtain the local concentration of free charge carriers. The method presented here therefore paves the way for a new quantum-enhanced electronic device technology, capable of mapping the interplay of mobile charges and electric fields in a working semiconductor device with nanometer precision.

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I. INTRODUCTION

The performance of semiconductor devices is crucially determined by the complex interplay between charge carriers and electric fields. Models that balance microscopic quantities, like, for instance, the formation of depletion zones or the distribution of free charge carriers, have allowed an in-depth understanding of the underlying physical processes to be obtained. Their validity was so far

mainly confirmed by comparing, for example, the resulting capacitance or current [1] as a function of the applied voltage, as electric fields and charge-carrier distributions inside the semiconductor are hardly experimentally accessible [2,3]. Electric fields originating from crystal defects can be mapped using the edge transient-current technique [4,5] but determining the local doping concentration remains challenging. Nevertheless, these models paved the way for one of the greatest technological advances in history: semiconductor electronics.

The described interplay takes mainly place in the depletion zones between p - and n -doped regions. An externally applied voltage on a p - or n -doped region leads to local changes in the band structure [see Fig. 1(a)], which is related to the spatial electric field E across the junction as

$$E = \frac{1}{e} \nabla \varepsilon_V(r). \quad (1)$$

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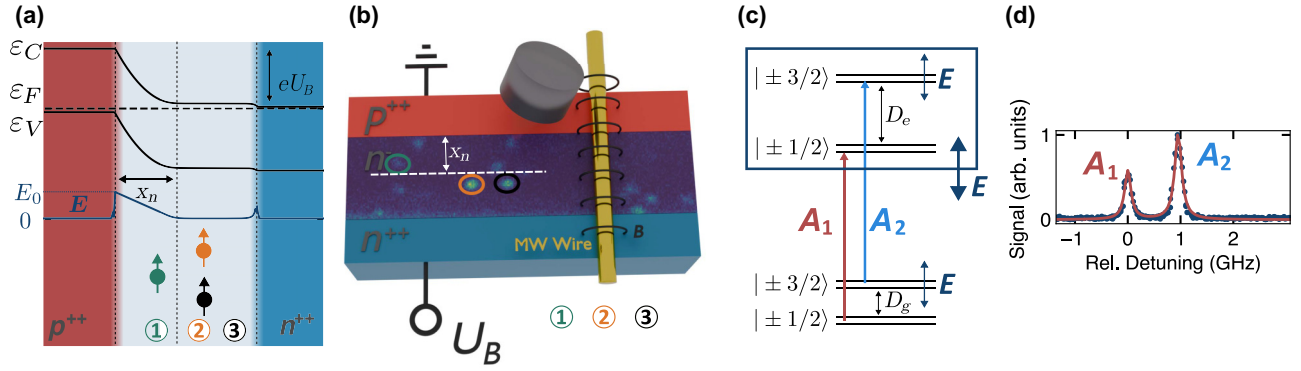


FIG. 1. (a) The properties of a semiconductor device, including the electric field E , are determined by its band diagram and can be extracted via operando measurements at various points inside the low n -type doped layer (further referred to as “intrinsic layer” of the p - i - n diode). At the interface between p^{++} and the intrinsic layer, a depletion zone of width x_n forms, which can be determined via measurements of various V_{Si} centers. (b) Schematic of our setup, composed of a 4H-SiC p - i - n diode, a microwave (MW) wire for spin manipulation, and a high-NA objective for excitation and collection of the emission. Color centers at a depth of approximately equal to $5 \pm 1 \mu\text{m}$ from the surface and different lateral positions inside the intrinsic region allow characterization of the semiconductor device, e.g., the extent of the depletion zone x_n . (c) Without a magnetic field, the $|\pm 1/2\rangle$ and $|\pm 3/2\rangle$ states are degenerate and connected to their excited states through A_1 and A_2 transitions. Axial electric fields influence both the ground (excited) state zero-field splitting D_g (D_e) as well as the zero-phonon-line between the ground and excited state with spin-dependent resonances A_1 and A_2 . (d) Both A_1 and A_2 transitions are identified via photoluminescence-excitation (PLE) measurements.

Here $\varepsilon_V(r)$ is the energy of the valence-band maximum and e the electron charge. It is therefore highly desirable to measure the electric field E with a high spatial resolution to gain a clear understanding of the device behavior.

It is only now that state-of-the-art quantum technology provides a way to microscopically investigate the interplay of electric fields and charges in a semiconductor component. For instance, wide-field N - V magnetometry allows the measurement of currents inside a photovoltaic cell, attached to a layer of N - V centers [6]. A color center, placed inside a device, can be used as a highly sensitive and robust quantum sensor to map electric fields [7,8] and charge densities. Such a quantum sensor offers the unique possibility to directly image an electric field and provides a quantitative estimation of charge carriers inside a device and—even more sophisticated—during operation. These insights are currently mainly accessed by numerical simulations. Obtaining them experimentally may deliver more detailed information about the critical influence of imperfections in real devices and hence has the potential to shift what is technologically possible.

For our experiments we use 4H-SiC, which is a well-established material for high-power semiconductor electronic applications [9]. In addition, 4H-SiC is also an excellent host material for quantum technology applications [10–12]. In particular, color centers inside the crystal lattice show excellent optical and spin properties [13–17], establishing them as an ideal platform for quantum communication [18,19], quantum computing [20–22], and quantum sensing [23–26]. Among the different color centers in 4H-SiC, the silicon vacancy (V_{Si}) center stands

out due to significantly reduced spectral diffusion [27], the integrability into nanophotonic devices [28], and long spin coherence times [29,30]. This makes the V_{Si} center a very promising candidate for quantum technology applications. A further advantage is the capability to integrate V_{Si} centers into semiconductor structures [25,31], which opens the unique possibility to monitor the interplay between electric fields and free charge carriers with nanometer resolution at various positions in an electronic device.

We show here the integration of single V_{Si} centers into a p - i - n diode [see Fig. 1(b)] for *in situ* and even operando mapping of electric field measurements and determination of the charge-carrier concentrations. For the measurements reported here spectroscopy of the V_{Si} center’s narrow optical resonances between the ground and excited state [see Figs. 1(c) and 1(d)] is performed and we find frequency shifts of their positions due to the Stark effect. Besides this, we show that the voltage-dependent onset of the Stark shift in correlation with the spatial position of a V_{Si} center enables spatially resolved monitoring of the formation of an electric field across the p - i - n diode [see Fig. 1(a)] and therefore, the local charge-carrier information. Our results mark an essential step towards an improved understanding of a semiconductor device, as the method presented here can be used at arbitrary locations inside the material and allows the physical parameters of the device to be inferred with nanometer resolution. Furthermore, we show that the voltage-dependent onset of the Stark shift is also present in optically detected magnetic resonance (ODMR) measurements. As ODMR is applicable at room temperature, the method presented here paves the way

for a new quantum-enhanced electric field mapping of semiconductor devices.

II. METHODS

The used p - i - n diode's n^{++} and p^{++} regions contain dopings in the range of $1 \times 10^{19} \text{ cm}^{-3}$ and are separated by a low n -type doped area of width $4.1 \text{ } \mu\text{m}$, which we denote in the following as the intrinsic region of the diode. Based on our Stark-shift measurements we find a concentration of dopants of around $9 \times 10^{14} \text{ cm}^{-3}$ (see discussion below), which deviates from the value specified by the manufacturer of $2 \times 10^{14} \text{ cm}^{-3}$. The single V_{Si} centers within the sample are created via electron irradiation followed by an annealing step. Further information about the sample can be found in Sec. S1 within the Supplemental Material [32]. Our measurements are carried out at room temperature and 5 K. Optical measurements are performed at 5 K with a home-built confocal microscope, where the optical resolution is diffraction limited at $> 500 \text{ nm}$. The sample is excited from a cleaved edge of the sample through a high-NA objective with a 730-nm laser for off-resonant and a tunable diode laser at 916 nm for resonant excitation. The emitted photons are filtered with a 950 nm long pass before being transmitted to a single photon detector with a quantum efficiency above 97% for the emission spectrum of the V_{Si} center. The manipulation of the spin states is realized by an arbitrary waveform generator and a microwave wire on top of the sample. Detailed information about the home-built confocal setup including Refs. [14,33–52] is shown in Sec. S2 within the Supplemental Material [32]. For our measurements, we use the k - V_{Si} center (V_2). The V_{Si} center

possesses a spin $S = 3/2$ with two spin-conserving optical transitions, denoted as A_1 and A_2 [see Fig. 1(c)]. These two resonances can be detected by optical spectroscopy of the V_{Si} center's fine structure, a method denoted as photoluminescence excitation (PLE) [Fig. 1(d)]. The energy of both optical transitions depends mainly on axial electric fields, which can be taken into account via the Stark-shift Hamiltonian [47,51]:

$$H_{\text{gs}} = (D + d_z E_z) S_z^2. \quad (2)$$

Here $2D = 70 \text{ MHz}$ is the zero-field splitting (ZFS) of the k - V_{Si} , which is shifted by an axial electric field E_z . S_z is the axial spin-3/2 operator in the reference frame of the V_{Si} center, where the z axis is defined by the c axis of the 4H-SiC lattice. Even though this Hamiltonian was derived for N- V centers in diamond, we do not expect changes for axial electric fields due to the C_{3v} symmetry of both N- V and V_{Si} centers. In Eq. (2) contributions of transverse electric fields can be neglected, as the electric field is aligned with the c axis of the crystal due to the device geometry, i.e., $E \parallel c$.

Equation (2) indicates that the axial electric field induced by the p - i - n diode leads to a Stark shift of the optical transitions A_1 and A_2 , which can be measured through PLE at cryogenic temperatures (5 K). An FEM simulation of the electric field under the Lorentz local field approximation in dependence of the applied voltage is shown in Fig. 2(a) [upper graph, further information about the FEM simulations can be found in Sec. S3 within the Supplemental Material [32]]. The electric field is generated by operating the p - i - n diode in reverse bias mode, where a positive voltage is applied on the n^{++} -doped area while the p^{++} layer is grounded. The local electric field E at

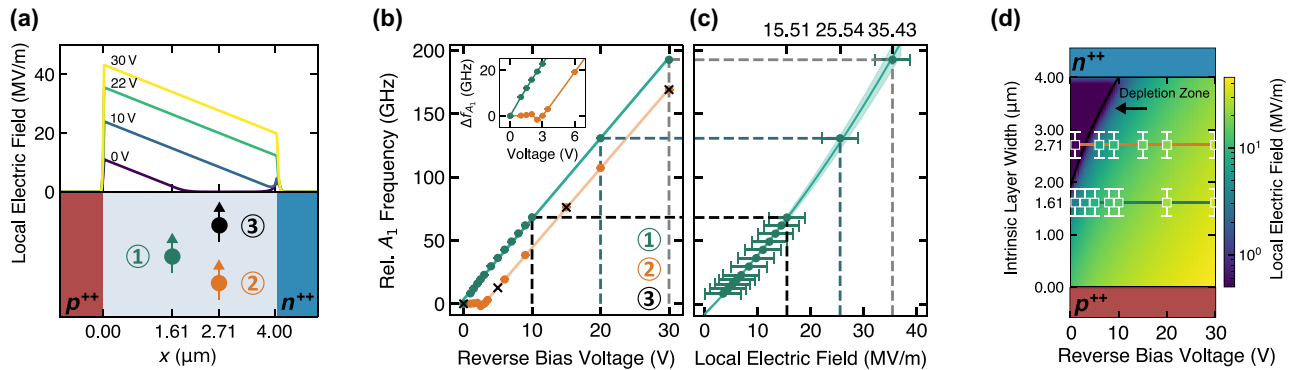


FIG. 2. 2D electric field mapping. (a) Local electric field, simulated across the intrinsic layer for voltages from 0 to 30 V, including the Lorentz local field approximation (see Sec. S3 within the Supplemental Material [32]). (b) Measured shift of A_1 lines upon different applied voltages. Inset: The relative shift of the A_1 frequency (Δf_{A_1}) of $V_{\text{Si}2}$ starts at around 2.6 V. (c) Stark shift of $V_{\text{Si}1}$ as a function of the local electric field, incorporating electric field uncertainty due to uncertainty of the V_{Si} position (horizontal error bars). The shaded region displays the fit with 1-sigma uncertainty. Measurements of the PLE frequency in (b) allow for the reconstruction of the electric field values. (d) Simulation of the electric field distribution in the intrinsic layer, indicating that for 0 V $V_{\text{Si}1}$ (green) is inside and $V_{\text{Si}2}$ (orange) outside the depletion zone (black line). Dopant concentrations as used in the simulations entering into (c),(d) is $9 \times 10^{14} \text{ cm}^{-3}$. Vertical error bars in (b),(c) are smaller than the data point.

the position of the V_{Si} centers within the intrinsic layer increases with the applied reverse bias voltage. In the lower graph [Fig. 2(a)], three V_{Si} centers are color coded at different positions in the intrinsic region (1.61 μm and 2.71 μm from the p^{++} layer) where the local electric field reaches values up to 35.43 MV/m for $V_{\text{Si}1}$ (28.04 MV/m for $V_{\text{Si}2,3}$) at 30 V. These V_{Si} centers are also shown with the same colors in the confocal map in Fig. 1(b).

III. RESULTS

We perform PLE measurements to determine the Stark shift caused by the electric field E within the intrinsic region. As can be seen from Fig. 2(b), the A_1 transitions are shifted with respect to the applied voltage and we find that the relative distance between the optical transitions of A_1 and A_2 stays constant at approximately 1 GHz (see Sec. S5 within the Supplemental Material [32]). The Stark shift of the $V_{\text{Si}1}$ center [marked green in Fig. 2(a)] increases linearly, but for $V_{\text{Si}2,3}$ centers (orange and black color code) the PLE frequency is only shifted for reverse bias voltages larger than approximately 2.6 V [inset Fig. 2(b)]. This behavior can be understood by considering the depletion from the p^{++} into the intrinsic layer, which scales as $x_n(V) \propto \sqrt{(V + V_{\text{BI}})/N_D}$, in terms of the built-in voltage $V_{\text{BI}} = 2.95$ V and N_D the concentration of dopants in the intrinsic layer. As $V_{\text{Si}2}$ is located 2.71 μm away from the p^{++} layer [Fig. 2(a)], the voltage-dependent extension of the depletion region can be used to infer the concentration of dopants in the intrinsic layer, which we find to

be $N_D = (8.7 \pm 2.2) \times 10^{14} \text{ cm}^{-3}$ (see Sec. S4 within the Supplemental Material [32] for the detailed calculation), resulting in a depletion region of $x_n = 1.9 \mu\text{m}$ for zero applied reverse bias voltage. This value is in good agreement with capacitance-voltage (C - V) measurements (see Sec. S1 [32]), yielding $N_D = 8.4 \times 10^{14} \text{ cm}^{-3}$. By simulating the electric field [Figs. 2(a) and 2(c)], the applied voltage can be converted into the resulting local electric field for $V_{\text{Si}1,2}$. The PLE shift is fitted with

$$\Delta f_{A_1} \propto -d \cdot E_z - \frac{\alpha}{2} E_z^2, \quad (3)$$

which allows to extract the dipole moment d and the polarizability α of $V_{\text{Si}1}$ as, respectively, $|d| = 4.33 \pm 0.15 \frac{\text{GHz}}{\text{MV/m}}$ and $\alpha = -0.09 \pm 0.01 \frac{\text{GHz}}{(\text{MV/m})^2}$ [Fig. 2(c)]. These values are in good agreement with the previously measured dipole moment of the k - V_{Si} of $d = 3.65 \frac{\text{GHz}}{\text{MV/m}}$ [53] and are comparable to first-principles estimates of the k - V_{Si} 's polarizability [37] and experimental measurements of hexagonal silicon vacancy (h - V_{Si}) centers [54]. A detailed discussion about the derived dipole moment and the polarizability can be found in Sec. S6 within the Supplemental Material [32]. Based on first-principles calculations, we determine $d = 1.83 \pm 0.01 \frac{\text{GHz}}{\text{MV/m}}$ and $\alpha = -0.0254 \pm 0.0006 \frac{\text{GHz}}{(\text{MV/m})^2}$ (see [32] for detailed information). The differences from our measured values are probably related to the functional used in the first-principles calculation and to piezo effects.

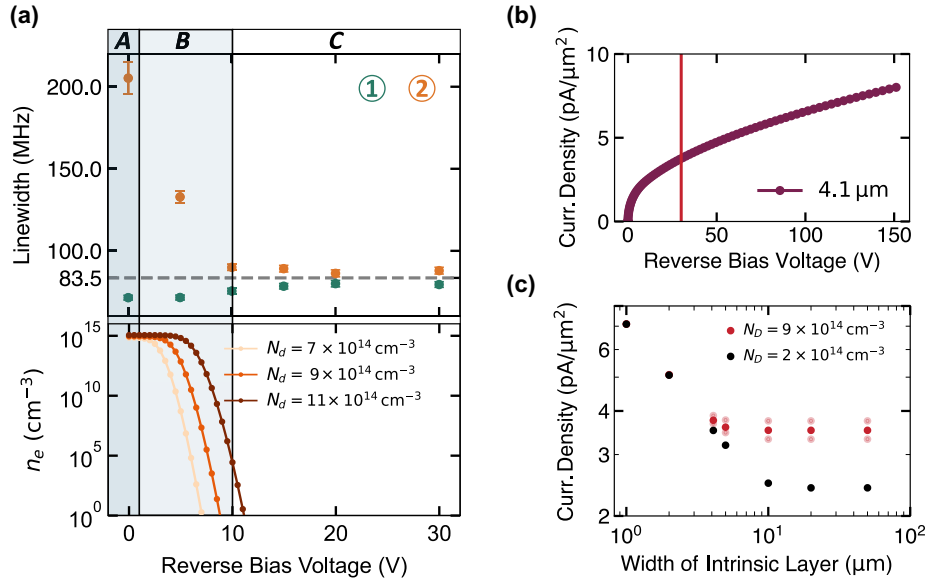


FIG. 3. (a) Dependency of the PLE linewidth on the position of the vacancy inside the intrinsic layer and the applied voltage. Upper panel: linewidth of $V_{\text{Si}1,2}$ centers as a function of applied reverse bias voltage. Lower panel: simulated concentration of electrons at the positions of $V_{\text{Si}1,2}$ centers. (b) Simulation of the reverse current density of the p - i - n diode considered here (width 4.1 μm , $N_D = 9 \times 10^{14} \text{ cm}^{-3}$) at different reverse bias voltages. (c) Simulation of the reverse current density at 30 V as a function of the width of the intrinsic layer for $9 \times 10^{14} \text{ cm}^{-3}$ (red) incorporating the uncertainty of the doping concentration (light red) and $2 \times 10^{14} \text{ cm}^{-3}$ (black).

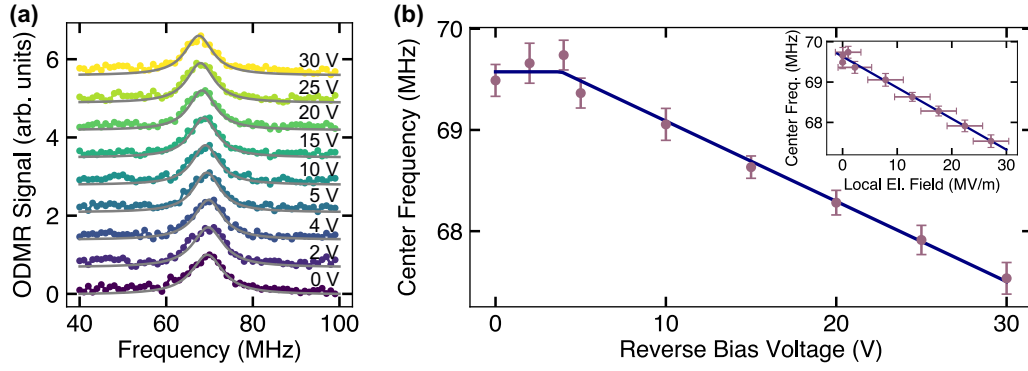


FIG. 4. (a) Off-resonant ODMR measurement for different applied reverse bias voltages of 0 V (blue) to 30 V (yellow), performed at room temperature. (b) The shift of the ODMR peaks reveals that only for voltages greater than 3.1 ± 2.4 V an effective field at the position of the vacancy forms, shifting the ZFS. Inset: shift of the ODMR center frequency as a function of the local electric field of V_{Si2} under the Lorentz local field approximation, revealing a gradient of $d_{GS} = -79.3 \pm 4.3 \frac{\text{Hz}}{\text{kV/m}}$.

The derived values of the dipole moment and polarizability are inherent properties of the V_{Si} center and are independent of the 4H-SiC device. For this reason, Stark-shift measurements of V_{Si} centers as a function of the applied reverse bias voltage allow for the reconstruction of the local electric field of the color center under consideration. This reconstruction is exemplarily performed in Figs. 2(b) and 2(c) for voltages of 10, 20, and 30 V, resulting in electric fields of, respectively, 15.03, 24.76, and 34.34 MV/m at the position of V_{Si1} . The presented measurement therefore opens the possibility to compare the measured electric fields against simulations of a semiconductor device [see data points in Fig. 2(d)]. The sensitivity of the measurements presented in Fig. 2 is $18 \frac{\text{kV/m}}{\sqrt{\text{Hz}}}$ (see Sec. S8 within the Supplemental Material [32]), which is comparable to single N-V centers [47] in bulk diamond. As the electric break-down field of typical SiC devices is on the order of 328 MV/m [55], V_{Si} centers are therefore excellent quantum systems to infer the mechanisms of the device failure, e.g., the electric-field-dependent onset of impact ionization [56].

Whereas the exact position of the PLE lines depends on the local electric field E seen by the single V_{Si} center, their optical linewidth is the result of charge fluctuations. Free charges can either stem from ionized defects, such as nearby ionized carbon vacancies [31], or incorporated dopants [57] residing in the vicinity of the V_{Si} center. The resulting electric field E_{fluc} created by the fluctuating charges couples to the permanent electric dipole moment d in the ground and excited state of the V_{Si} as $H \sim d \cdot E_{fluc}$. Therefore, the optical linewidth depends on the fluctuating electric field around the V_{Si} and a reduction of mobile charges in the local environment of the V_{Si} center causes a reduced optical linewidth of both A_1 and A_2 . This can be achieved within a p - i - n diode due to the formation of a depletion region by applying reverse bias voltages [46]. We find that the optical linewidth

strongly depends on the position of the color centers and can range from 205.2 ± 9.8 MHz to 71.5 ± 1.4 MHz in the absence of any applied reverse bias voltage, as shown in Fig. 3(a). We attribute this behavior to the width x_n of the depletion region in the absence of an applied reverse bias voltage. As the sample's built-in voltage of $V_{BI} = 2.95$ V causes the depletion zone to extend $1.9 \mu\text{m}$ into the intrinsic layer, V_{Si1} [$x = 1.6 \mu\text{m}$, see Fig. 2(a)], resides in the space-charge region of the diode, contrary to V_{Si2} ($x = 2.7 \mu\text{m}$). This indicates that—unlike V_{Si2} —the charge environment around V_{Si1} center is initially already depleted. An increase of the reverse bias voltage of the p - i - n diode shifts the depletion region further into the intrinsic area where eventually also the V_{Si2} center is in the space-charge region. As a consequence, the concentration of surrounding charges around V_{Si2} is significantly reduced and the optical linewidth starts to narrow. If the reverse bias voltage is increased ≥ 10 V, the optical linewidth of the V_{Si2} center reaches its plateau of approximately 80 MHz. This finding stays in good agreement with the charge-depletion simulation shown in Fig. 3(a) (bottom), indicating that free charges within the intrinsic region are fully depleted at a reverse bias voltage of ≥ 10 V.

Whereas the linewidth of the V_{Si2} center decreases with increasing reverse bias voltage, the linewidth of the V_{Si1} center gets broadened [see Fig. 3(a) region B], which cannot be explained by the depletion of free charges within the intrinsic area. Based on FEM simulations of the p - i - n diode, it can be shown that with increasing applied reverse bias, a reverse current starts to flow [see Fig. 3(b)]. This behavior is in accordance with I - V measurements of our p - i - n diode (see Sec. S1 within the Supplemental Material [32]). This reverse bias current causes a rise of mobile charge carriers flowing in the vicinity of the V_{Si1} center and therefore increases its optical linewidth. As the concentration of charges due to this current is on the order of approximately 10^8 cm^{-3} (see Sec. S9 [32]), the broadening

effect is small compared to the narrowing effect of the formation of the space-charge region (which reduces the charge concentration by approximately 10^{15} cm^{-3}). It can be seen from Fig. 3(a) (region C) that $V_{\text{Si},2}$ centers both approach a linewidth of around 80 MHz for high voltages. Here both V_{Si} are in the space-charge region and the same current flows nearby. This linewidth is larger than the V_{Si} center's A_2 optical lifetime limit of 14 MHz [48], which we attribute to the reverse current becoming the dominant mechanism at higher voltages. It should be emphasized, that the effective reverse bias current might deviate from Fig. 3(b) due to imperfections of the studied p - i - n diode (see Sec. S1 within the Supplemental Material [32] for additional discussion). As discussed in Sec. S10 within the Supplemental Material [32], we do not expect magnetic fields originating from reverse currents to influence the PLE measurements reported in this paper. Simulations show that the reverse current can be minimized by using an intrinsic layer with a reduced concentration of dopants as well as an intrinsic region with a width of $\geq 10 \text{ }\mu\text{m}$ [Fig. 3(c)]. The PLE linewidth can additionally be reduced with an improved epitaxial layer quality, which reduces deep traps and thus prevents Shockley-Read-Hall generation [58] of charges and a structured p^{++} layer minimizing edge currents (see discussion in Sec. S1 within the Supplemental Material [32]).

To extract the influence of the reverse bias voltage onto the ground state of the $V_{\text{Si},2}$ center, we performed ODMR measurements at room temperature for reverse bias voltages from 0 V up to 30 V [see Fig. 4(a)]. There is a clear shift of the resonance position from the ZFS of approximately 70 MHz visible within the measurements, which is in good agreement with ODMR simulations based on Eq. (2) (see Sec. S10 within the Supplemental Material [32]). This shift is in very good agreement with resonant ODMR measurements as shown in Sec. S10 [32]. For this reason, the electric field at the position of $V_{\text{Si},2}$ has the same strength at room and cryogenic temperatures. As the ground state of V_{Si} centers has no temperature dependence [26], we exclude the ZFS shifts as shown in Fig. 4 to originate from heating of the device due to the reverse current. The strength of the shift correlates with the applied reverse bias voltage and a gradient of $d_{\text{GS}} = -79.3 \pm 4.3 \frac{\text{Hz}}{\text{kV/m}}$. The electric field across the p - i - n diode is oriented from the n^{++} to the p^{++} side, which is parallel to the quantization axis of the V_{Si} center. Our measurements therefore allow not only the absolute value of the electric field to be inferred, but also whether it is aligned in parallel with the c axis (0001 direction) or rotated by 180° with respect to the c axis (000-1 direction). The onset of the Stark shift, which has been seen in Fig. 2(b) at around 2.6 V, is also present in these ODMR measurements [Fig. 4(b)]. This method therefore allows the expansion of the depletion region to

be extracted based on the applied reverse bias voltage at ambient temperature.

IV. CONCLUSION

In conclusion, we have shown the local-measurement-based reconstruction of physical parameters in an electronic device, like the formation of the space-charge region, the electric field, and the doping level with V_{Si} centers in 4H-SiC. The presented method allows the measurement of device characteristics with an Abbe-limited lateral spatial resolution of approximately 500 nm, even far below the surface and at various positions within the semiconductor device. Silicon-vacancy centers are also excellent sensors of, e.g., temperature [25,59] and magnetic fields [24,60], where the latter can be used to infer the current density in operating integrated circuits [61] with operation regimes from cryogenic up to very high temperatures [62]. We envisage that V_{Si} centers enable the full operando monitoring of semiconductor devices, which can greatly help to infer the device performance characteristics and improve their performance in power electronics. Besides this, the presented method can also contribute to a better understanding of charge-carrier concentrations at low temperature.

Besides applications in the electrometry of semiconductor devices, the method presented here is also of great use to establish silicon-vacancy-based quantum communication networks. These protocols rely on indistinguishable photons emitted from separate quantum network nodes. This can be achieved by utilizing the presented p - i - n diodes, whose resonances are tuned such that the emitted photons have the same wavelength and two-photon interference [63,64] can occur, which is a prerequisite for spin-spin entanglement [65,66].

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D.S. fabricated the p - i - n sample and carried out the I - V measurements. F.H. performed the PLE and ODMR measurements. F.H. and M.H. performed the sensitivity measurement. J.S. performed the FEM simulations of the p - i - n diode and carried out the C - V measurement. W.K. irradiated the sample. P.U. performed the simulations of the dipole moment and polarizability. H.W. supported sample manufacturing. M.H. performed the data analysis, the ODMR and PLE simulations, wrote the manuscript and coordinated the project. R.N. supervised the project. All authors discussed and contributed to the manuscript.

The authors declare no competing interests.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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