

Vanadium photoluminescence in 3C-SiC

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Early investigations on vanadium in the cubic 3C-SiC polytype concluded that the luminescence of the center is not possible because the excited state is degenerate with the conduction band. However, later work refuted this notion, demonstrating a doublet in photoluminescence (PL) at ~ 1493 – 1495 nm, apparently associated with vanadium (V). In this work, we undertake a detailed experimental and theoretical study of the V center in 3C-SiC. We show that the vanadium PL can be seen as a recombination of an exciton bound to V, in contrast to the other two common hexagonal polytypes (4H- and 6H-SiC), where the PL is due to an interatomic transition of the $3d$ electron within the V center, according to a well-established model. We also show that the splitting observed in the PL lines is likely not inherent to the center and is due to stress present in the samples. Ideally, in a strain-free 3C-SiC material, the vanadium PL will comprise a single line, which makes the V center in this polytype attractive for applications as a qubit at moderate temperatures. This contrasts with the hexagonal polytypes where the splitting of the zero-phonon line is inherent to the center due to the crystal structure, which has a negative effect on the spin coherence at liquid helium temperature, and millikelvin temperatures are needed to improve the spin coherence.

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I. INTRODUCTION

Vanadium substituting for a Si atom in the hexagonal 4H- and 6H-polytypes of SiC is a well-studied amphoteric impurity that can compensate both n - and p -type materials, yielding semi-insulating properties [1–3]. Deep-level transient spectroscopy (DLTS), the temperature-dependent Hall effect, photoelectron paramagnetic resonance (photo-EPR), and optical measurements have been used to establish the charge transition levels (CTLs) of V within the band gaps of 4H- and 6H-SiC [2–9]. However, the band-gap positions of the donor and acceptor levels of V present in the literature

show a significant spread for both hexagonal polytypes. The acceptor-level ($0|$) positions with respect to the conduction band edge (CBE) E_C range from $E_C - 0.62$ to $E_C - 0.78$ eV for 6H-SiC (from $E_C - 0.8$ to $\sim E_C - 1.1$ eV for 4H-SiC) in different works, while for the donor level ($+|0$), the scatter is in the range $E_V + 1.35$ to $E_V + 1.7$ eV for 6H-SiC ($E_V + 1.54$ to $E_V + 1.78$ eV for 4H-SiC) with respect to the valence band edge (VBE) E_V [3]. Arguably, the most plausible values for the donor level in 4H- and 6H-SiC are approximately $E_V + 1.6$ eV, and for the acceptor levels in 4H- (6H-SiC) – approximately $E_C - 0.97$ eV ($E_C - 0.85$ eV) [3,10,11]. Although V in 4H- (6H-SiC) has two (three) inequivalent configurations corresponding to the inequivalent Si lattice sites in the unit cell (hexagonal or quasicubic), the site dependence of the CTLs is rarely resolved. Therefore the above values should be considered as approximate generic values. One exception is the work of Lauer *et al.* [12], in which the authors claim to resolve the hexagonal site from the cubic sites for the V ($0|$) CTLs (i.e., V^{3+}) in 6H-SiC, $E_C - 0.74$ and $E_C - 0.68$ eV, respectively.

It is well known that the neutral charge state of V (V^{4+}) with one $3d$ electron [$V(3d^1)$] has an excited state (ES) within

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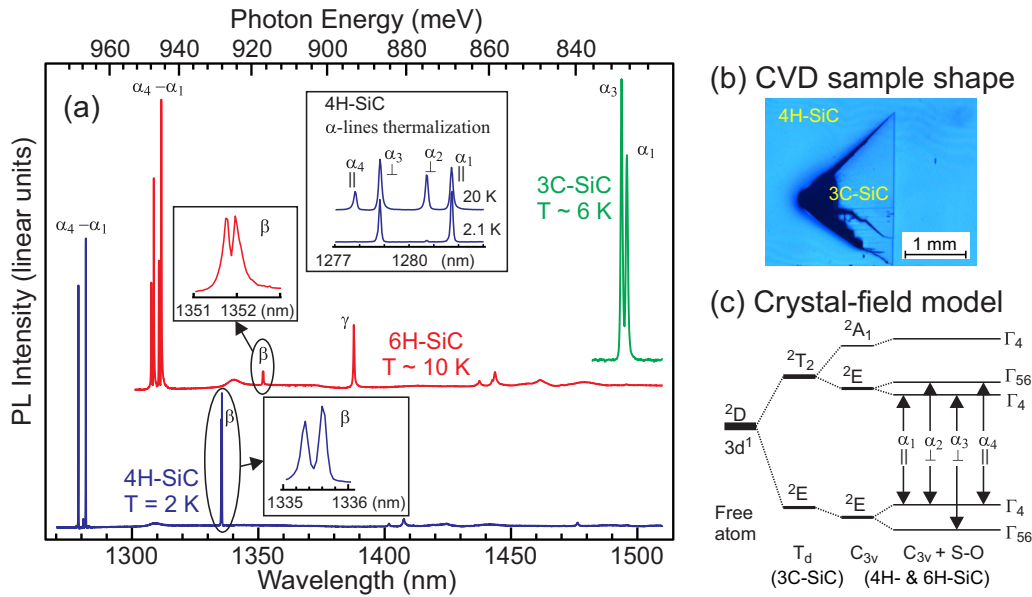


FIG. 1. (a) Comparison of the PL signatures of V in 4H-, 6H-, and 3C-SiC, as denoted for each spectrum. The inset at the top shows the thermalization of the α lines in 4H-SiC: the α_2 and α_4 lines appear only at higher temperatures because they originate from the higher component of the excited state. The line polarization is also shown ($\parallel$ - parallel to the crystal c axis, $\perp$ - perpendicular to it). The two lower insets zoom into the splitting of the β lines in 6H- and 4H-SiC. (b) Photograph of the triangular 3C-SiC inclusion in the 120- μm thick CVD-grown 4H-SiC epilayer. (c) Schematic energy diagram adapted from [14] showing the splitting of the fivefold degenerate $3d$ -electron term when the symmetry is lowered from spherical to T_d (the symmetry of V in 3C-SiC), and further to C_{3v} (specific for 4H- and 6H-SiC). Further splitting is due to spin-orbit interaction (S-O) in the hexagonal polytypes, but not in 3C-SiC.

the band gaps of 4H- and 6H-SiC and, therefore, emits light upon optical excitation [3,4,12,13]. The emission for both hexagonal polytypes is in the telecom O band with the lowest-energy γ line of 6H-SiC in the E-band, spanning the range 1278–1388 nm (0.89–0.97 eV). The electronic structure and optical properties of V($3d^1$), i.e., V^{4+} , have been studied both experimentally and theoretically [14,15], and an excellent agreement between the experiment and the phenomenological theory based on the crystal field model of V($3d^1$) electron in 6H-SiC has been demonstrated [14]. The neutral vanadium possesses electron spin 1/2, and its applicability as qubit in spintronics has been tested recently [11,16,17].

The cubic polytype 3C-SiC doped with vanadium has also been investigated [18,19]. In the earlier work of Dombrowski *et al.* [18], it is argued that the photoluminescence (PL) of V in 3C-SiC is not present because due to the smaller band gap of the cubic polytype the ES is degenerate with the conduction band (CB). However, later work demonstrated sharp PL lines in V-doped 3C-SiC, which are apparently related to V [20]. This first experimental observation of vanadium PL has been confirmed in our present work on a series of sublimation-grown 3C-SiC. The results are complemented with measurements on vanadium-doped epitaxially grown 3C-SiC in the form of macroscopic triangular inclusions embedded in a 4H-SiC matrix. The experimental results and the discussion of a plausible model for the V PL in 3C-SiC are the subject of the present article. In Sec. II, we present the experimental details and describe the samples. Section III first presents the experimental results and afterwards considers the experiment in the light of the model considered previously [18] and a new model developed by us in which the vanadium

PL can be viewed as due to exciton recombination at the defect. We also present the results of first-principles calculations corroborating our model. Section IV summarizes the conclusions.

II. METHODS

A. Experimental details

The two types of samples used in this study are grown either by sublimation or by chemical vapor deposition (CVD). The sublimation-grown samples are thick (up to 1 mm) 3C-SiC crystals grown on the Si face of 4H-SiC off-axis substrates using a lateral enlargement growth technique described elsewhere [21,22]. The vanadium doping is implemented using V-doped source powder. About a dozen samples were grown, all of which show essentially the same spectrum related to V in 3C-SiC as illustrated in Fig. 1(a). The epitaxial sample is grown using chemical vapor deposition (CVD) on standard 4H-SiC 4° -off cut Si-face substrate. The V doping is implemented by adding to the gas system H_2 gas passing through liquid VCl_4 , as described in Ref. [23]. The cubic polytype forms as macroscopic triangular inclusions grown in the 4H-SiC epitaxial film of 120 μm thickness, as illustrated in Fig. 1(b). The V doping concentration measured by secondary ion mass spectrometry in the 4H-SiC epilayer on this sample is $2 \times 10^{14} \text{ cm}^{-3}$ and is assumed to be similar to that in the 3C-SiC inclusion if the incorporation rates of V in 3C- and 4H-SiC are similar.

The PL measurements are performed by cooling the sample in a variable temperature closed-cycle cryostat (Montana S50). An Ar-ion laser emitting at 488 nm is used for

excitation with estimated power at the sample below 1 mW. The laser is focused, and the emitted PL is collected by a microscope objective of magnification 50X and numerical aperture 0.7. The laser spot diameter is $\sim 2 \mu\text{m}$. The PL is detected with a monochromator (Jobin Yvon model HR460) equipped with a multichannel InGaAs detector with nearly constant quantum efficiency in the range 800–1590 nm. The spectral resolution of the system using 300 grooves/mm grating and the typical 50 μm slit opening is $\sim 0.4 \text{ nm}$ ($\sim 0.2 \text{ meV}$).

For the Raman measurements, we use a 2400 grooves/mm grating which provides $\sim 0.05 \text{ nm}$ resolution with 50 μm slit. We use an excitation of 532 nm from a solid-state laser. This configuration enables distinguishing shifts in the Raman lines well below 1 cm^{-1} (the pitch between the CCD-camera pixels corresponds to $\sim 0.28 \text{ cm}^{-1}$). For the lifetime measurements, the sample was excited by $\sim 200 \text{ ps}$ pulses of a diode laser emitting at a wavelength of 440 nm at a repetition rate of 1 MHz and an average power of $45 \mu\text{W}$. The PL signal was bandpass-filtered (12 nm FWHM, centered around 1490 nm) and analyzed by time-correlated single photon counting using a superconducting single photon detector and time-tagging electronics.

B. Computational details

The calculation of vanadium doping in 3C-SiC is implemented by employing the Vienna *ab initio* simulation package (VASP 5.4.1) code within the framework of density functional theory (DFT) [24–27]. The Heyd–Scuzeria–Ernzerhof (HSE) hybrid functional and related HSE06 parameters are used for accurate predictions of defect levels [28–30]. Vanadium (V) substituting at the silicon atomic site is modeled in a 512-atom 3C-SiC supercell ($4 \times 4 \times 4$) with Γ -point sampling in the Brillouin zone. The cut-off energy is set at 420 eV, which is suitable for all elements. The geometry relaxation convergence conditions are set to 10^{-4} eV and $-0.01 \text{ eV/\AA}$ for the total energy and force thresholds. To correct for an inaccuracy of the HSE functional caused by an overscreening of localized states, d-orbitals of V, the on-site correction (HSE + V_W) is applied [31,32] with value of $V_W = -2.5 \text{ eV}$ [31]. The excited state is constructed by using the ΔSCF approach [33] to promote one electron from an occupied localized Kohn-Sham (KS) level to a higher unoccupied one.

III. RESULTS AND DISCUSSION

A. Comparison of the V-related PL in 4H-, 6H-, and 3C-SiC

Figure 1(a) shows an overview of the low-temperature spectra of the V-related PL in the three common polytypes 4H-, 6H-, and 3C-SiC. The three (two) inequivalent lattice sites in 6H- (4H-SiC) give rise to three (two) defect centers, denoted with α , β , and γ in 6H-SiC and α and β in 4H-SiC. Earlier work has assigned the α lines in 4H- and 6H-SiC to the hexagonal lattice sites and the rest of the lines to the (quasi)cubic sites. This assignment is due to the apparent resemblance of the α lines in both polytypes (the GS and the ES are both well resolved doublets giving rise to a four-line manifold) and the fact that both polytypes have only one hexagonal site, while 4H-SiC has one cubic and 6H-SiC two

cubic sites. However, later work has reviewed this assignment and associated the α lines in 4H-SiC with the cubic site [15].

The argument provided in Ref. [18] is developed as follows. The authors measure the electron paramagnetic resonance (EPR) spectra under illumination with monochromatic light of different energies in *p*-type 3C-SiC. The spectrum of the neutral V^{4+} is barely observable for photon energies below $\sim 1.7 \text{ eV}$ but strongly enhanced above this energy, which is interpreted as conversion of the positive charge state V^{5+} into the neutral one by photoexcitation of a valence band electron to the $V (+|0)$ level. Further, they use the V donor level ($+|0$) as a common reference in 6H- and 3C-SiC, as suggested by the Langer-Heinrich rule [34]. If the threshold for the conversion $V^{5+} \rightarrow V^{4+}$ is indeed 1.7 eV , using the low-temperature band gap of 3C-SiC of 2.416 eV [35], we obtain that the energy distance between the $(+|0)$ level of V [the ground state (GS) of the neutral V^{4+} impurity] and the CBE is approximately 0.72 eV . Hence, an ES of $\sim 0.83 \text{ eV}$ (or more) above the GS would fall within the CB. However, the experimental observation of the V-related emission around 0.83 eV in 3C-SiC [20] (cf. also Fig. 1) suggests a lower position of the $(+|0)$ level with respect to the VBE. Indeed, another publication [6] contemporary with [18] uses optical admittance spectroscopy (OAS) to investigate the $V (+|0)$ level position, quoting the value 1.59 eV below the CBE in 6H-SiC. Using the band-gap value of 3.083 eV for this polytype [36], we obtain for the position of the $(+|0)$ V level $\sim 1.5 \text{ eV}$ above the VBE. This is to be compared with the value of 1.6 eV obtained by Maier *et al.* [7] by photo-EPR for the same polytype. Furthermore, while the value of 3.1 eV for the band gap of 6H-SiC obtained in [6] is in excellent agreement with the value of 3.083 eV determined on the ground of the excitonic band gap and the free exciton binding energy [36], the value for the 4H-polytype is overestimated in OAS, 3.41 eV to be compared with the 3.286 eV determined optically [37]. On the other hand, the *ab initio* calculation results presented in Sec. IIIC yields 1.54 eV above the VBE for the position of the $(+|0)$ V level, however, the calculated band gap of 3C-SiC is underestimated (2.23 eV) yielding only 0.69 eV between the $(+|0)$ level and the CB edge. Thus one may anticipate that the values obtained by photo EPR and OAS are not very accurate, and both techniques may have an error margin in the range $0.1\text{--}0.2 \text{ eV}$. Similar error margin is anticipated for the first-principles calculations. Therefore we may conclude that the experimental data presented above does not have sufficient accuracy to unambiguously determine whether the position of the excited state is in the CB or below it.

There are, however, two indirect hints suggesting that the ES of V in 3C-SiC is in the CB. Indeed, firstly we notice from Fig. 1 that the α and β lines are shifted in 4H- and 6H-SiC by $\sim 20\text{--}30 \text{ meV}$ and together occupy the region $891\text{--}970 \text{ meV}$. On the other hand, the doublet associated with the V emission in 3C-SiC appears at substantially lower energy ($\sim 828 \text{ meV}$), well-separated from the 4H- and 6H- ZPLs. This suggests that the energy separation between the GS of V and the CB edge is not large enough to accommodate an ES-GS transition of energy $\sim 0.9 \text{ eV}$, and in the next section, we present an alternative excitonic model for V PL in 3C-SiC. The second tip for the different nature of the PL of V in 3C-SiC comes from the

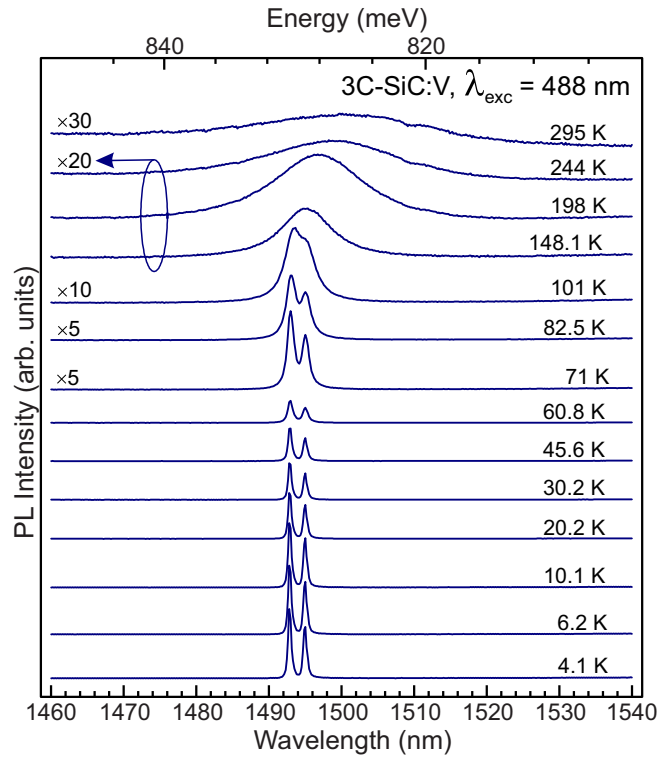


FIG. 2. Temperature dependence of the V-related PL spectrum in 3C-SiC. The two zero-phonon lines at ~ 1493 and 1495 nm show a constant intensity ratio before merging in a single band due to the temperature-induced line broadening. The spectra demonstrate that the V emission persists up to room temperature. Notice the scale changes in the spectra.

temperature dependence presented in Fig. 2. If we assume for the moment that the ES of V is within the band gap of 3C-SiC, it should be quite close to the CB edge. This anticipation is based on the Langer-Heinrich's rule [34] suggesting at least 1.5 eV above the VBE for the GS of V and the observed transition energy of ~ 0.83 eV. Therefore the ES would exhibit phonon-assisted ionization at high enough temperatures and the PL for the defect should vanish with increasing temperature, similar to the phonon-assisted ionization of the ES of the *divacancy* in 3C-SiC [38]. However, the PL of V in 3C-SiC remains observable up to room temperature, which also suggest a different mechanism for this luminescence.

It is worth noting here that using EPR detected via magnetic circular dichroism (MCD-EPR) Dombrowski *et al.* [19] observe an *absorption* line at essentially the same energy position (0.828 eV) as the PL peaks of Ref. [20]. In Ref. [19], no PL from V is observed, possibly due to poor sample purity leading to many nonradiative recombination channels quenching the PL. We notice in addition, that for a defect with ES degenerate with the CB it is unlikely to observe either PL or sharp absorption related to the GS-ES transition of this defect.

We also notice here that the PL reported in [20] is a well-resolved doublet (cf. Fig. 1), while the absorption peak observed in Ref. [19] shows no splitting. We will demonstrate later that the splitting of ~ 1.2 meV observed in many samples in PL is most likely adventitious and due to strain, especially prominent in the set of sublimation-grown by lateral enlarge-

ment samples of 3C-SiC on an off-axis 4H-SiC substrate [21,22].

B. Crystal-field model of V in 3C-, 4H-, and 6H-SiC and excitonic model of V PL in 3C-SiC

The free V atom has the electronic configuration $[\text{Ar}] 3d^3 4s^2$. When occupying a Si site in SiC, four of the five valence electrons form bonds with the four tetrahedrally coordinated nearest C neighbors. The fivefold degeneracy of the remaining one $3d$ electron level is split by the crystal field and possible spin-orbit interactions in the corresponding polytype, as illustrated in Fig. 1(c). The model originally proposed in Ref. [14] illustrates the splitting of the $3d$ level when the symmetry of the V-atom environment is lowered from spherical in the free atom to tetrahedral T_d in the cubic 3C polytype, and to C_{3v} in the hexagonal polytypes. V^{4+} has electron spin $1/2$ (the electron terms are doublets), therefore, in C_{3v} symmetry a further splitting of the ^2E level occurs into Γ_4 and Γ_{56} levels due to the spin-orbit interaction. Here, we use the notations of Ref. [14] for the extra irreducible representations Γ_4 and $\Gamma_{56} = \Gamma_5 \oplus \Gamma_6$ of C_{3v} .

Thus, the PL related to V in the hexagonal polytypes stems from $\Gamma_4 \leftrightarrow \Gamma_{56}$ transitions between the GS and the ES manifolds, as denoted by arrows in Fig. 1(c) and well-illustrated for the α sites in 4H- and 6H-SiC (cf. Fig. 1). However, in T_d symmetry pertinent to 3C-SiC, there is no orbital momentum associated with either the ES ($^2T_2$) or the GS (^2E), hence, there is no spin-orbit splitting. Thus the theoretical prediction is that a single line should be observed from V in 3C-SiC if the PL transition is between the $^2T_2$ and ^2E states. (In fact, as discussed below, most likely the $^2T_2$ is indeed degenerate with the CB of 3C-SiC and the V PL in 3C-SiC can be viewed as an exciton recombination at the V center rather than an interatomic transition.) Furthermore, the temperature dependence of the V spectrum shown in Fig. 2 demonstrates that the two split-off components of the ZPL do not thermalize, which means that the splitting is in the GS, ^2E . However, the GS should not split in T_d symmetry. This apparent inconsistency was puzzling at first since the splitting suggests lowered symmetry of the defect, and a possible symmetry lowering due to the Jahn-Teller effect would not explain such a small splitting. Another reason for the symmetry lowering could be strain (uniaxial or biaxial), and later we present convincing evidence that this is the real reason for the observed splitting.

We now consider qualitatively the excitonic model for the PL of V in 3C-SiC, which assumes that the ES $^2T_2$ of the $3d$ electron is degenerate with the CB. In the next section, we present the results of *ab initio* calculations on the V defect in 3C-SiC, confirming that the ES is degenerate with the CB and corroborating the notion of recombination of an exciton bound to the V center. Already now we can notice that the V ZPLs in 4H- and 6H-SiC (about and above 0.9 eV in energy) are well separated from the ZPLs of 3C-SiC (0.83 eV), which is an indirect indication that an interatomic transition with energy similar to that of the hexagonal polytypes ($> \sim 0.9$ eV) does not fit within the band gap of 3C-SiC, as discussed in Sec. III. A (cf. also Fig. 3). We can then conclude that Ref. [18] is correct in assuming the ES $^2T_2$ is degenerate with the CB,

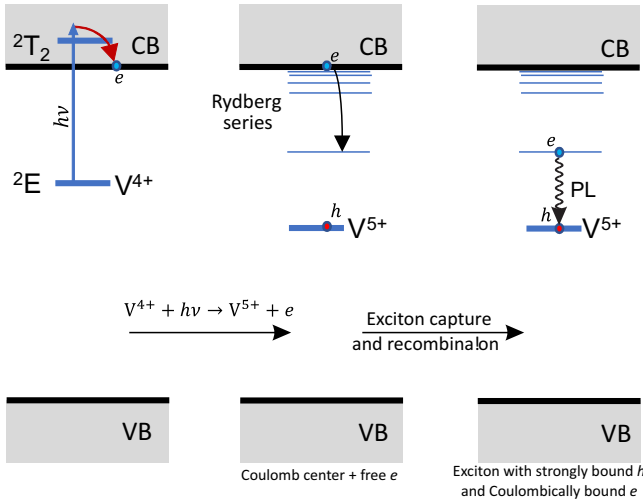


FIG. 3. Schematic presentation of the exciton capturing mechanism for V in 3C-SiC using one-particle energy diagrams. The left panel presents the photoexcitation of the $3d$ electron in the CB. A Coulomb center (V^{5+}) is created, and the free electron is captured to one of the states of the Rydberg series (mid panel). In the right panel, the electron relaxes to the lowest excited state of the Rydberg series, and subsequent recombination with the V-bound hole gives rise to the PL.

hence no luminescence due to ${}^2T_2 \leftrightarrow {}^2E$ transitions can be observed. However, another possibility exists for a radiative transition associated with the V center. In a previous work [39], it is argued that a defect with charged states within the band gap is always capable of binding an exciton. Applied to V in 3C-SiC, the following mechanism schematically presented in Fig. 3 can be envisaged. First, the $3d$ electron of V is excited in the CB by absorption of a photon of energy $h\nu$ larger than the energy difference between the CBE and the V^{4+} level, leaving the V center in the positively charged V^{5+} state plus a free electron (denoted e in Fig. 3):

$$V^{4+} + h\nu \rightarrow V^{5+} + e.$$

Thus, a Coulomb center is created (V^{5+}), in the corresponding Coulomb field of which the free electron will be captured. This hydrogen-atom-like system possesses an infinite set of ESs (Rydberg series) converging towards the CB. One of these *excited* states has the lowest energy and the captured electron will rapidly thermalize into that state. This system can be viewed now as an exciton bound to the V atom with a strongly bound hole (the missing electron in V^{5+} , denoted h in Fig. 3) and a coulombically bound electron. The recombination of the bound exciton is the origin of the PL observed from V in 3C-SiC. We notice that schematic energy diagrams shown in Fig. 3 should be treated with some caution because we attempt to depict two particles, electron (e) and hole (h), using a one-particle energy diagram. Nevertheless, the mechanism of binding an exciton is understandable from the presented description.

The results from the calculations from first principles done for the V center in 3C-SiC are described in the next section.

C. Results from the first-principles calculations

The calculated band gap of pristine 3C-SiC is 2.23 eV, showing proper folding of the X point in the applied supercell where the conduction-band minimum (CBM) resides in the Brillouin zone. Upon introducing vanadium doping, we find that in the neutral charge state only a single spin-polarized, double-degenerate e state appears within the band gap, while all other localized levels lie within the conduction band. The calculated ($+|0\rangle$) charge-transition level lies 1.54 eV above VBM, in excellent agreement with experimental findings. As the empty t_2 defect level lies in the conduction band, the ${}^2T_2$ excited state of V^{4+} is resonant with the conduction band. Consequently, the electronic configuration of the lowest energy excited state can be described as a localized hole on the in-gap e level and an electron split from the CBM, i.e., a bound exciton. Using the Δ SCF approach, where an electron is promoted from the e level to the CBM, we obtain a raw zero-phonon line (ZPL) energy of 0.55 eV, which increases to 0.65 eV after applying the charge correction [40]. This value still falls below the experimental ZPL of approximately 0.8 eV, likely reflecting an underestimated band-gap value that is 0.19 eV smaller than the experimental reference. Additionally, strain in the experimental samples may shift the defect levels, contributing to the observed discrepancy.

Regarding the splitting of the PL peak in the spectrum, we analyze how strain-induced symmetry reduction affects the splitting of the degenerate ground-state energy levels, i.e., the e KS levels constituting the ${}^2E$ ground state. Firstly, we demonstrate the effect of uniaxial strain on the degenerate KS levels, where strain induces a distortion in the crystal and reduces the total symmetry from T_d to D_{2d} point symmetry. The uniaxial strain is applied by changing the x component of the lattice constants in the Cartesian coordinate system (which contains three orthogonal vectors: x , y , and z , where $|x| = |y| = |z| = a$ of the face-centered cubic system) with a smeared occupation of electrons on the two e KS levels as follows:

$$\begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{bmatrix} \rightarrow \begin{bmatrix} a(1 + \varepsilon) & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{bmatrix},$$

where ε is an element of the introduced uniaxial strain coefficient matrix. The uniaxial strain will cause a splitting of the e KS levels, as shown in Fig. 4(a). The splitting (ΔE) shows a linear relationship with ε , and the slope is 3287.9 (303) meV/strain. In practice, the strain is on the order of 10^{-4} (~ 0.33 meV according to our simulation), which is close to the peak-splitting values in the experimental PL spectra (~ 0.38 versus 1.17 meV).

Additionally, we consider also shear strain leading to C_{3v} symmetry of V in 3C-SiC. Under this point-group symmetry, spin-orbit coupling (SOC) occurs in the ground state, and the axial component of the SOC also leads to a ${}^2E$ level splitting. A shear strain matrix is applied to the cubic lattice constant matrix to distort the geometry from T_d to C_{3v} point symmetry, as shown below

$$\begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & a \end{bmatrix} \rightarrow \begin{bmatrix} a & \varepsilon a & \varepsilon a \\ \varepsilon a & a & \varepsilon a \\ \varepsilon a & \varepsilon a & a \end{bmatrix}.$$

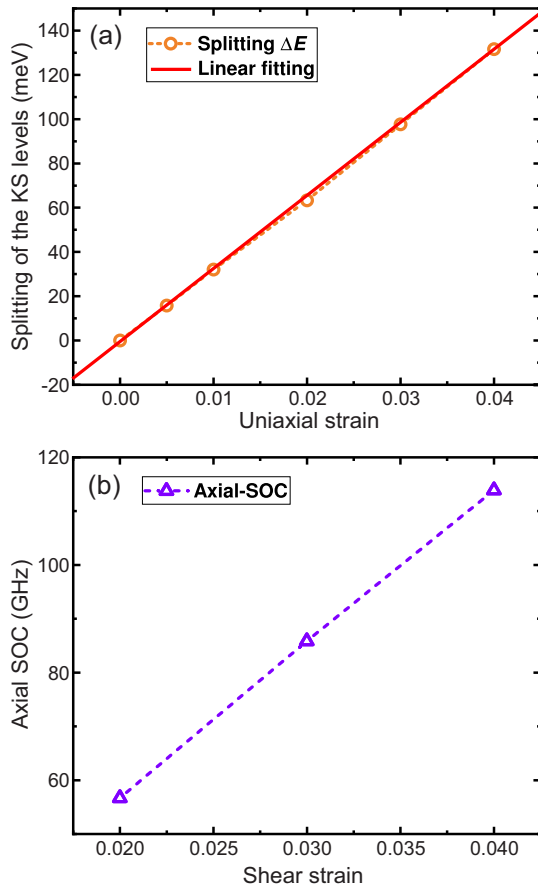


FIG. 4. The calculated strain effect on the degeneracy of ^2E KS levels in the ground state. (a) The ^2E KS level orbital splitting under D_{2d} point symmetry caused by uniaxial strain. The red line represents a linear fit. (b) The ^2E KS level spin-orbit splitting caused by axial SOC under C_{3v} symmetry when shear strain is present.

The calculation employs a noncollinear approach [41] implemented in VASP, based on the Perdew–Burke–Ernzerhof (PBE) functional [42], with verified accuracy in our previous works [43,44]. The splitting due to SOC is illustrated in Fig. 4(b). From Fig. 4(b), when the strain increases from 2% to 4%, the SOC increases from 57 to 114 GHz splitting, i.e., from 0.23 to 0.47 meV, with a slope of $k_{C_{3v}} = 11.8$ (1) meV/strain, which is much smaller than the splitting caused by uniaxial strain. In practical situations, a strain of about 10^{-4} would cause a negligible splitting of ~ 0.0012 meV).

In summary, our calculations indicate that the most likely reason for splitting of the two ZPLs in the PL spectrum is symmetry reduction induced by uniaxial strain splitting the degeneracy of the orbital ^2E levels in the GS, and effects of possible shear strain can be disregarded.

D. Photoluminescence results

In Sec. III A, we compared the PL spectra related to V in the three common polytypes, 4H-, 6H-, and 3C-SiC (cf. Fig. 1). In Sec. III B, we argued that while in 4H- and 6H-SiC, the PL excitation-luminescence cycle can be viewed as an interatomic transition between crystal-field and valley-orbit-interaction split-off levels of the vanadium 3d electron, in

3C-SiC the most plausible scenario is that the luminescence is due to recombination of a V-bound exciton. However, the ground state into which the system relaxes after the emission of a PL photon is the ^2E ground state. The latter is subject to splitting due to spin-orbit interaction in the hexagonal 4H and 6H polytypes, but not in the 3C-SiC polytype, as mentioned in Sec. III B. On the other hand, the temperature dependence of the V spectrum in 3C-SiC shown in Fig. 2 demonstrates no thermalization of the two sharp-line components. Their ratio remains nearly constant with temperature, suggesting that the splitting is in the ground state of the center. It is worth mentioning that our first spectra obtained from a set of about ten V-doped samples grown by the same sublimation method as described in Refs. [21,22] always showed the same low-temperature spectrum of V, with about the same line positions (~ 1493 and 1495 nm) and the same splitting of ~ 1.2 meV between the two components. Since no ground-state splitting is expected for this defect with anticipated T_d symmetry, we were led to assume symmetry lowering, which, judging from the repeatability of the spectra from all sublimation samples, is inherent to this particular set of samples. The two possible reasons for symmetry lowering are the Jahn-Teller effect and uniaxial or biaxial strain, of which only the Jahn-Teller effect can be inherent to the defect, whereas the strain is an external (adventitious) effect. However, the possibility that all sublimation-grown samples are subject to the same stress conditions due to the specific growth technique (essentially, heteroepitaxial growth of single-domain 3C-SiC on 4H-SiC substrate), leading to the same splitting in PL, cannot be entirely excluded. Therefore, it is important to compare the spectrum from the sublimation-grown samples to the spectrum of V from a 3C sample grown by a different method where the stress conditions typical for the sublimation growth cannot be repeated. We found such different samples in the form of macroscopic ($\sim 1 - 2$ mm) triangular 3C-SiC inclusions embedded in 4H-SiC V-doped thick epitaxial layers (~ 120 μm thick) grown by CVD with controlled nitrogen and vanadium doping (concentrations $[N] \approx 1 \times 10^{15} \text{ cm}^{-3}$, $[V] \approx 2 \times 10^{14} \text{ cm}^{-3}$).

Figure 5 compares two spectra from each of the two types of samples. The spectrum from the CVD-grown sample (top curve) appears upshifted in energy by ~ 2 meV from that of the sublimation-grown sample. The splitting into two components can still be clearly discerned, however, its value has diminished by a factor of 3 compared to the other sample (~ 0.38 versus 1.17 meV). Both the spectral shift and the diminished splitting demonstrate that the splitting is not an inherent effect but adventitious due to strain in the samples. We notice that the spectrum for the CVD sample is measured near the top (the tip) of the elevated formation on the 3C triangular island [corresponding to the middle of the dark area near the left-hand corner of the triangle in Fig. 1(b)]. Other spectra measured on different points within the triangle together with spectra from sublimation samples are presented in Ref. [45]. The PL spectra indicate variation of the strain conditions in different samples and even in different points within the same sample leading to variations in the splitting magnitudes and the line positions. See Ref. [45] for further observations on the inhomogeneous distribution of the strain in the samples.

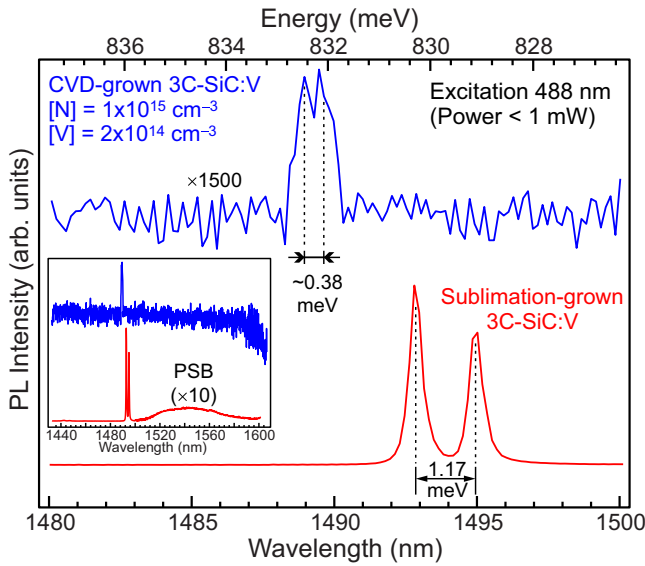


FIG. 5. Comparison of the structure of the ZPL spectrum of V in the two types of samples used in this study, CVD grown (top curve) and sublimation grown (bottom). The inset shows the full spectrum, including the PSB, which is well visible for the sublimation sample. Note the change of the scaling factor for the PSB. The difference in intensity between the two samples (~ 3 orders of magnitude) is believed to be largely due to the difference in vanadium concentrations.

We note that the PL signal in the CVD-grown sample is much weaker than that in the other sample, possibly due to the lower V concentration (the V concentration in the sublimation-grown sample is unknown but likely in the high 10^{16} cm^{-3} range) and, possibly, the relatively higher nitrogen concentration leading to that many of the V centers may be in the negative (dark) state. For that reason, the spectrum had to be recorded with a somewhat lower resolution [100 μm monochromator slit ($\sim 0.8 \text{ nm}$ resolution) instead of 50 μm], and the phonon sideband (PSB) is not discernible. However, it is worth noting that the PSB which is easily detected in the sublimation-grown sample is relatively weak, hence the Debye-Waller factor of the center is among the high ones compared to other defects (e.g., the silicon vacancy or the divacancy in 4H- and 6H-SiC), albeit we do not attempt to estimate it here (cf. the inset in Fig. 5, notice the magnification factor for the PSB).

Photoluminescence excitation efficiency. The spectra presented so far for V in 3C-SiC are recorded with an excitation wavelength of 488 nm from an Ar ion laser. Since the Ar ion laser visible lines span across the electronic band gap of 3C-SiC (2.416 eV at 2 K [35]), it was interesting to observe the effect on the PL of excitation energies below and above the band gap. We use the Ar-laser lines in the range 457.9 nm (2.707 eV)–514.5 nm (2.409 eV), of which the latter laser line has energy below the electronic band gap. The results are shown in Fig. 6. Apparently, above-band-gap excitation is much more efficient in exciting the vanadium PL. An analogous effect has been observed for the V emission in 4H-SiC, where above-band-gap excitation (351 nm from an Ar-ion laser) has been observed to have at least three orders of magnitude higher efficiency in exciting the V PL compared

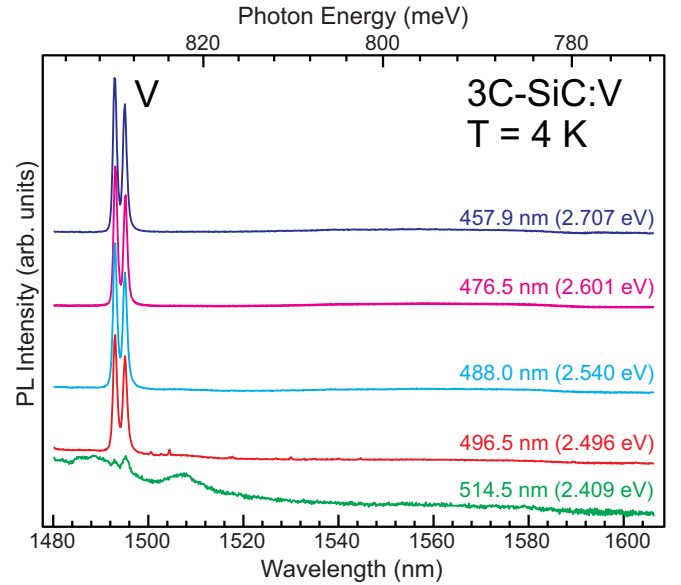


FIG. 6. PL spectra of V in the 3C-SiC sublimation sample excited with different photon energies, both above and below the electronic band gap. The spectra illustrate an abrupt drop in excitation efficiency for below-band-gap excitation.

to below-band-gap excitation at 514.5 nm ([46], the 351-nm excitation data is unpublished). Thus, for both polytypes, 3C- and 4H-SiC, the experimental data indicate very efficient exciton capture and inefficient “photon capture,” i.e., small absorption cross-section for below-band-gap-energy photons. This situation may arise if the V-center has large capture cross-section for holes (free, or nearly-free as in an exciton), whereas the very weak absorption cross-section for below-band-gap photons can be associated with the very weak appearance of the phonon sideband for V (true also for the 4H- and 6H-SiC polytypes), possibly due to weak electron-phonon coupling compared to other defects. However, further theoretical work needed for a better understanding of the excitation mechanism is deemed beyond the scope of this paper. The observed phenomenon is not fully understood at present, but it seems that the creation of free excitons associated with above-band-gap excitation and their subsequent capture to the V centers provides the most efficient excitation mechanism in both 3C- and 4H-SiC. More comprehensive PL excitation studies are necessary to shed light on the excitation properties of V in various SiC polytypes.

Photoluminescence lifetime. We measured the PL lifetime at low temperatures (5 K), and from the fit of the one-exponential decay data, we obtained the value of $1.065 \pm 0.002 \text{ ns}$ in the sublimation-grown sample (see Sec. S2 in Ref. [45]). However, it should be noted that this lifetime is likely quenched due to the presence of impurities and other defects, which create nonradiative recombination channels. The exciton-recombination model would suggest a significantly longer lifetime owing to the relatively small overlap of the wave functions of the Coulombically bound electron and the tightly bound hole. Lifetime measurements on the epitaxially grown sample were not successful due to the low count rate.

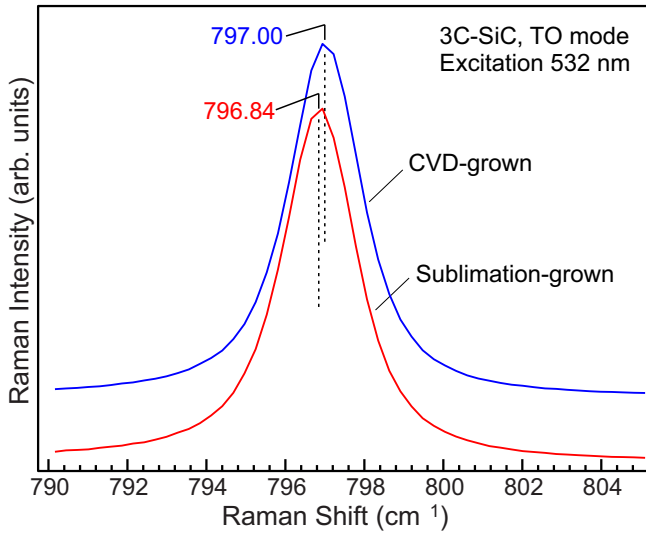


FIG. 7. Expanded view of the Raman spectra of the two 3C-SiC samples in the vicinity of the TO mode, illustrating the TO downshift in the sublimation sample compared to the CVD sample. The spectra are typical representatives near the tip of the CVD sample and in the region of the sublimation sample where the PL spectra of Fig. 5 are measured. The spectra are recorded under the same conditions without moving the monochromator grating between the measurements to prevent accidental shifts in the calibration wavelength.

The PL spectra do not allow us to conclude whether the stress present in the samples is compressive or tensile. That is why we use high-resolution Raman spectroscopy to obtain information about stress.

E. Raman spectroscopy

The Raman spectrum of 3C-SiC exhibits only two modes, TO and LO (at ~ 796 and 972 cm^{-1} , approximately [47]). We compare the positions of the TO mode on different spots of several samples, including CVD- and sublimation-grown. We use the TO mode because the LO mode couples to plasmons, and its position is influenced by variations in the electron concentration. Some results from the measurements for the two samples used in Fig. 5 are presented in Fig. 7. More data are shown in Fig. S3 in Ref. [45]. Comparing the two samples in Fig. 7, the TO mode of the CVD sample is upshifted with respect to that of the sublimation sample. Although the spectra from different points on the samples presented in Fig. 7 show some scatter of the TO-mode positions, it seems that the TO mode of the CVD sample is upshifted with respect to that of the sublimation sample. There is no information about the character of the strain: uniaxial, biaxial, or a mixture of both (from the geometry of the samples uniform hydrostatic strain is unlikely to occur and can be safely disregarded). However, it is natural to assume that the smaller splitting in the PL lines near the tip of the CVD sample corresponds to less strain than in the sublimation sample, and since TO peak in the former is upshifted with respect to the TO peak in the latter sample, we assume that larger tensile strain in the sublimation sample is the cause for larger splitting compared to the CVD sample. We need to remark here that both tensile and compressive strains have been reported for triangular inclusions of 3C-SiC em-

bedded in CVD-grown 4H-SiC epilayers [50,51]. Our results suggest that at least near the top of the elevated region on the CVD sample the strain is relaxed (smaller PL splitting) and the strain in the sublimation sample is larger than that in the CVD sample and tensile because the TO peak is downshifted in frequency. It is worth noticing, however, that the maximum observed shifts of the TO mode across all measured spots on all the samples are on the order of one pixel ($\sim 0.3\text{ cm}^{-1}$, cf. Ref. [45]), whereas the PL-line positions seem to be much more sensitive to strain. Due to the lack of an unstrained reference sample, however, we can only compare the relative shifts in the samples investigated.

However, the character of the strain is most likely different in both types of samples because of their different geometries. The sublimation growth is done by lateral enlargement of a 3C seed in one direction, suggesting that uniaxial strain is likely present in the sample. In the case of triangular 3C inclusions in the CVD-grown 4H samples, a strain that is closer to biaxial would be expected. Results from simulations using finite-element calculations of the strain in CVD-grown samples similar to those used in the present study are available [51], suggesting on the order of 100–200 MPa of stress near the center of a triangular 3C inclusion embedded in a 100- μm -thick 4H-SiC epilayer at the growth temperature of 1923K. However, this work predicts compressive strain at the elevated growth temperature, albeit it is possible that a compressive strain in the triangle transforms into tensile (or weaker compressive) strain at measurement temperature near the tip of the elevated region where the spectrum in Fig. 5 is measured. The same work indicates that the stress decreases with increasing epilayer thickness. The notion of decreasing strain near the tip of the CVD sample is further corroborated by comparing Raman spectra measured near the tip and on the surface of the triangle (see Fig. S3 in Ref. [45]). Finally, we estimate the order of the expected strain using literature data from *hydrostatic* stress measurements. Hydrostatic stress (pressure) of $\sim 100\text{ MPa}$ leads to an upshift of the TO mode of $\sim 0.5\text{ cm}^{-1}$ [52]. This corresponds to roughly 4×10^{-4} of strain, which is in good agreement with the values quoted in the theoretical Sec. III C. This estimate should only be considered accurate to within an order of magnitude because the stress in our samples is not hydrostatic. To conclude, the small shifts observed in the TO mode between the samples and between different points on the same sample are consistent with the magnitude of strain ($\sim 10^{-4}$) predicted from the theory to account for the observed splitting of the V PL line in 3C-SiC.

IV. CONCLUSION

We have identified the PL signature of V in 3C-SiC and suggested as underlying physical mechanism recombination of an exciton bound to the V center, in contrast to the interatomic transition producing the luminescence from V in the hexagonal 4H- and 6H-SiC polytypes. We thus refute the suggestion of previous work that the V-related PL in 3C-SiC is degenerate because the excited state (the $^2T_2$ level) is degenerate with the CB. The results of the first-principles calculation confirm that the $^2T_2$ level is degenerate with the CB due to the smaller band gap of 3C-SiC and agree with the

model of bound-exciton recombination. Our work also reveals that the reason for splitting in the V-related PL lines is the strain present in the samples, which leads to the lowering of the symmetry of the defect. If high-quality V-doped strain-free 3C-SiC was available, the observed PL should consist of only a single peak associated with the ^2E ground state, in contrast to the doublet inherent to the hexagonal polytypes (4H- and 6H-SiC) due to the ground-state splitting by spin-orbit interaction into Γ_4 and Γ_{56} components. This makes the use of the V defect in 3C-SiC for qubit applications advantageous to the use of V in the hexagonal polytypes because the lack of spin-orbit splitting in the ground state eliminates the possibility for an Orbach process in the ground state [53,54], which would degrade the spin-lattice relaxation time unless millikelvin temperatures are employed. Indeed, long spin relaxation times have been observed for V in 4H-SiC, but a temperature of 100 mK–1.3 K has been used in these measurements [17]. The applicability of the V defect in 3C-SiC for quantum applications still remains to be explored.

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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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