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Splitting of type-I (N-B, P-Al) and type-II (N-Al, N-Ga) donor-acceptor pair spectra in 3C-SiC

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Discrete series of lines have been observed for many years in donor-acceptor pair (DAP) spectra in 3C-SiC. In this work, the splitting of both type-I (N-B, P-Al) and type-II (N-Al, N-Ga) DAP spectra in 3C-SiC has been systematically investigated by considering the multipole terms. For type-I spectra, in which either N or B substitutes on C sites or P and Al replace Si, the splitting energy of the substructure for a given shell is almost the same for both pairs. For type-II spectra, in which N is on the C site while Al and Ga acceptors replace Si, we find that, when compared with literature data, the splitting energy for a given shell is almost independent of the identity of the acceptor. For both type-I and type-II spectra, this splitting energy can be successfully explained by the octupole term V_3 alone with $k_3 = -2 \times 10^5$ Å^4 meV. Comparing the experimental donor and acceptor binding energies with the values calculated by the effective-mass model, this suggests that the shallow donor (N,P) ions can be treated as point charges while the charge distribution of the acceptor ions (Al,Ga,B) is distorted in accord with the T_d point group symmetry, resulting in a considerable value for k_3. This gives a reasonable explanation for the observed splitting energies for both type-I and type-II DAP spectra.

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I. INTRODUCTION

In the past few years, important developments in the growth technique for cubic silicon carbide (3C-SiC) have renewed interest in it for electronic device applications.[1] Thus, understanding and characterizing impurities due to residual or intentional doping provides important feedback for the crystal growth and device fabrication. To this end, low-temperature photoluminescence (LTPL) spectroscopy has proved for a long time to be a most convenient and nondestructive technique for the detection and identification of optically activated impurities.[2–6] Basically, in SiC, the group-V substitutional impurities (nitrogen and phosphorus) are donor species while all group-III atoms are acceptors. Among them nitrogen, which is by far the most common residual donor, substitutes on the carbon sites.[2] On the contrary, based on the size of its covalent radius,[2] phosphorus is expected to substitute preferentially on the silicon sites. The group-III substitutional impurities (Al, Ga, and B) are all potential acceptors and, among them, Al and Ga substitute on the Si sites while B has been demonstrated to reside on C sites,[6] although some authors believe that it may occupy also Si sites.[2] When both the donor and acceptor substitute on the same sublattice, they give a type-I donor-acceptor pair (DAP) spectrum while, if they reside on the two different sublattices, the spectrum is called type II. In 3C-SiC, both N-B and P-Al DAP spectra have been recognized as type I (because N and B substitute on the same carbon sublattice and P and Al on the silicon one). In the case of N-Al and N-Ga DAP spectra, they have both been recognized as type II.

Compared to the other acceptors, Al gives the shallowest acceptor level while B gives the deepest one in all SiC polytypes. Usually, residual N and Al species are the most common donor and acceptor species in 3C-SiC.[3] They are then often identified from the unambiguous observation of specific donor-acceptor-pair transitions in the LTPL spectra.[4] Concerning DAP spectra involving the nitrogen donor, apart from the N-Al recombination lines, N-Ga and N-B DAP spectra have also been observed in 3C-SiC.[4–7] Concerning phosphorus, the experimental results are more scarce and only P-Al DAP spectra have recently been identified.[8] The subject of interest in this work is to analyze the discrete lines in the DAP spectra, which are due to close-pair recombination spectra.[4–8]

The analysis of these sharp (discrete) lines yields important information on the host material and the impurities. This includes the dielectric constant,[9] the van der Waals interactions,[10] and the ionization energies of the donor and acceptor species.[5,8,11] This analysis is based on the formula[12]

$$h\upsilon(R) = E_g - (E_D + E_A) + E_C - E_{vdW}, \qquad (1)$$

in which $h\upsilon(R)$ is the energy of the photon emitted from a DAP with separation R, E_g is the band gap energy, E_D and E_A are the donor and acceptor ionization energies, and E_C is the Coulomb interaction energy between the donor and acceptor ions after recombination. Finally, E_{vdW} is the van der Waals (vdW) interaction energy between the neutral donor and neutral acceptor atoms before recombination. The sharp lines in the high-energy part of the DAP spectra are assigned to the recombination of close DAPs at distances R, which take on the set of discrete values permitted by the lattice structure. The shell number m is then used to identify the order of these discrete lines depending on R. However, for a given m, some of the lines can further split into several components.

In the first approximation, assuming that the donor and acceptor behave as *point* charges after recombination and point dipoles before recombination, one can get E_C as

$$E_C = \frac{e^2}{4\pi\varepsilon_0\varepsilon R},$$

while the van der Waals term is given by[10]

$$E_{vdW} = \frac{e^2}{4\pi\varepsilon_0\varepsilon R}\left(\frac{b}{R}\right)^5.$$

In these expressions, e is the electron charge and ε the dielectric constant. After identification of the values of R corresponding to the different shell numbers m, the observed DAP lines can be fitted by Eq. (1) and such a fit yields a rather accurate value for $h\upsilon(R \to \infty) = E_g - (E_D + E_A)$.[4–7,12] However, as mentioned above, in both type-I and type-II DAP spectra, some of the shell lines are further split into well-resolved components. This cannot be explained by Eq. (1) and one has to go a step further.

Moving beyond this first approximation, Patrick[13] introduced in 1968 a multipole correction to the Coulomb potential to explain the shell splittings observed in the DAP line spectra of GaP. The shell substructure was associated with the presence of inequivalent sets of lattice sites for the same shell number.[11–13] In the zinc-blende structure, the charge of the donor and acceptor ions has a spatial extension with a shape determined by the T_d point group symmetry. The correction to the Coulomb energy of a donor ion in the multipole field of an acceptor, and vice versa, is then given by the first nonvanishing multipole terms in the cubic field, V_3 and V_4:[11,12]

$$V_3 = \frac{k_3 xyz}{R^7}, \tag{2}$$

$$V_4 = \frac{k_4(x^4 + y^4 + z^4 - 0.6R^4)}{R^9}. \tag{3}$$

The coefficients k_3 and k_4 are unknown parameters, evaluated by fitting the shell substructure of spectra.[13,14] In this way, for GaP, considering all DAP spectra which involve the deep O donor together with the C,[13] Zn,[14] or Cd (Ref. 15) acceptors, the shell substructure splitting could be satisfactorily described by Eqs. (2) and (3). For the O-C results, the spectra gave $k_3 = \pm 2.4 \times 10^5$ Å^4 meV and $k_4 = 0$.[13] For the O-Zn spectra, $k_3 = -2.4 \times 10^5$ Å^4 meV and $k_4 = 1.9 \times 10^6$ Å^5 meV were found.[14] Finally, for O-Cd specta, $k_3 = -2.4 \times 10^5$ Å^4 meV and $k_4 = 2.8 \times 10^6$ Å^5 meV were obtained.[15] From these results, it was suggested that k_3 is mainly deep donor dependent and k_4 shallow acceptor dependent.

In 3C-SiC, Choyke and Patrick fitted the N-Al DAP line spectrum in the region of rather high shell numbers ($30 < m < 44$). However, in this region very few shells exhibit measurable line splittings, namely, the shells with $m =$ 31, 32, and 40 (see Fig. 2 of Ref. 4), because for such large shell numbers the splittings of the lines belonging to the same m are typically well below 0.5 meV. On the contrary, the composing lines for each shell in the region of $8 \leqslant m \leqslant 17$ can be clearly resolved either in the N-Al spectrum shown here or in that of Ref. 4. The only exception is the shell with $m = 10$. It should have two components (corresponding to 24 and 4 atoms in two subshells), but the weak component (4 atoms) has not been identified in all type-II spectra, probably because it falls within one of the surrounding stronger lines. In this work, we follow Patrick's method and consider both type-I (N-B, P-Al) and type-II (N-Al, N-Ga) DAP spectra in 3C-SiC. We find that the splitting energy for a given shell is almost independent of the type of donor and the acceptor species involved, but, of course, the line structure depends on the type of DAP spectra. Thus, in both cases of type-I and type-II spectra the splitting of the shell substructure can be successfully described by considering the multipole term V_3 with $k_3 = -2 \times 10^5$ Å^4 meV [Eq. (2)].

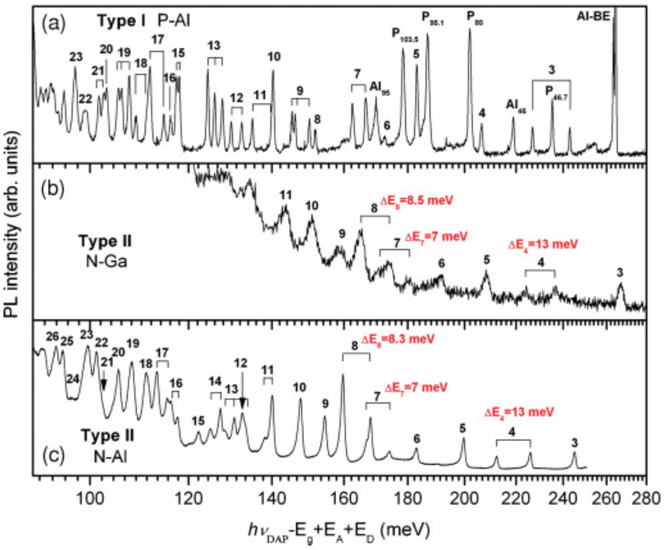

FIG. 1. (Color online) LTPL spectra of type-I (P-Al) and type-II (N-Al, N-Ga) spectra in 3C-SiC. The shell numbers m are also given for each shell. As examples, the splitting energies for $m = 4,7,8$ are also given by $\Delta E_4 = 13$, $\Delta E_7 = 7$, $\Delta E_8 = 8.3$ meV for both N-Al and N-Ga spectra, respectively.

II. EXPERIMENT

A. Type I spectra

The first experimental observation of type-I DAP spectrum in 3C-SiC was reported by Kuwabara *et al.*[6] in 1976. In Ref. 6, N and B co-doping was done with both of them residing on the C site. The experimental spectrum is shown in Fig. 1 of Ref. 6 and, to the best of our knowledge, constitutes the only report available for N-B DAP spectra in 3C-SiC so far. The experimental spectra are not so well resolved and not all substructures can be clearly identified. More recently, a well-resolved series of line substructures was found in P-Al DAP spectra in 3C-SiC.[8] This is shown in Fig. 1(a). The splitting energy for a given shell is compared between N-B and P-Al in Table I.

B. Type II spectra

In Figs. 1(b) and 1(c), as examples, we show N-Al (sample S1) and N-Ga (sample S2) DAP spectra in 3C-SiC. The detailed growth conditions of these two samples can be found in Ref. 7. LTPL spectra were collected at 5 K using a frequency-doubled Ar$^+$-ion laser for excitation ($\lambda = 244$ nm). The nominal (incident) power was ~30 mW and a Jobin Yvon-Horiba Triax 550 spectrometer, fitted with a 2400 grooves/mm grating and a cooled CCD camera, completed the setup. To complement the splitting data we also compare our data with N-Al results of Ref. 4 and the N-Ga data of Ref. 5 in Table II.

TABLE I. Comparison of the calculated splittings ($\Delta E = 2|V_3|$) of type-I DAP substructures and observed values in 3C-SiC. The observed splitting energy ΔE is obtained from the difference between the neighboring lines within the same shell. Shells, inequivalent sets of lattice vectors $\langle uvw \rangle$ in units of $\frac{1}{2}a_0$ for a given shell, and the number of sites for equivalent sets of the same shell are also listed between $m = 3$ and 23. The calculation was performed using $k_3 = \pm 2 \times 10^5$ Å^4 meV. The P-Al and the N-B DAP data are from Refs. 8 and 6, respectively.

Shell m	$\langle uvw \rangle$ ($\frac{1}{2}a_0$)	Number of sites	V_3 (meV)	ΔE(meV) Calculated	ΔE(meV) Observed P-Al (Ref. 8)	ΔE(meV) Observed N-B (Ref. 6)
3	$\pm\langle 211 \rangle$	12 + 12	33.473	66.9	16.2	–
4	$\langle 220 \rangle$	12	0	0	–	–
5	$\langle 310 \rangle$	24	0	0	–	–
6	$\pm\langle 222 \rangle$	4 + 4	11.834	23.7	–	10.1
7	$\pm\langle 321 \rangle$	24 + 24	5.175	10.3	4.1	4.2
8	$\langle 400 \rangle$	6	0	0	–	–
9	$\pm\langle 411 \rangle$	12 + 12	1.431	2.9	0.8	0.9
9	$\langle 330 \rangle$	12	0	0	3.9	3.4
10	$\langle 420 \rangle$	24	0	0	–	–
11	$\pm\langle 332 \rangle$	12 + 12	3.191	6.4	4.7	3.6
12	$\pm\langle 422 \rangle$	12 + 12	2.092	4.2	2.5	1.7
13	$\pm\langle 413 \rangle$	24 + 24	1.185	2.4	1.8	2.4
13	$\langle 510 \rangle$	24	0	0	1.7	–
15	$\pm\langle 512 \rangle$	24 + 24	0.598	1.2	0.7	–
16	$\langle 440 \rangle$	12	0	0	–	–
17	$\pm\langle 433 \rangle$	12 + 12	1.39101	2.8	2.8	1.7
17	$\langle 530 \rangle$	24	0	0	–	–
18	$\pm\langle 442 \rangle$	12 + 12	1.012	2.0	2.0	1.8
18	$\langle 600 \rangle$	6	0	0	–	–
19	$\pm\langle 532 \rangle$	24 + 24	0.785	1.6	1.5	1.4
19	$\pm\langle 611 \rangle$	12 + 12	0.157	0.3	0.6	0.9
20	$\langle 620 \rangle$	24	0	0	–	–
21	$\pm\langle 541 \rangle$	24 + 24	0.368	0.7	0.8	0.7
22	$\pm\langle 622 \rangle$	12 + 12	0.376	0.7	0.6	–
23	$\pm\langle 631 \rangle$	24 + 24	0.241	0.5	0.4	–

III. RESULTS AND DISCUSSION

A. Type-I spectra

In a type-I DAP spectrum, there is a characteristic doublet substructure with a splitting which only depends on the octupole term V_3. Thus, we first will fit the data of type-I spectra in 3C-SiC. In Table I we take the origin at a donor (acceptor) site and define $\langle uvw \rangle$ as the set of sites obtained by applying all the operations of T_d to an acceptor (donor) site $[uvw]$. Units of $\frac{1}{2}a_0$ are used for u, v, and w to avoid fractions. The sets $\langle uvw \rangle$ and $-\langle uvw \rangle$, hereafter labeled as $\pm\langle uvw \rangle$, are inverse (inequivalent) sets unless one or two of u, v, or w is zero. This is the origin of the characteristic doublet splitting coming from the octupole term V_3. Obviously, the term V_4 does not give any contribution to the splitting of doublets. This makes the fitting of splitting energies for type-I spectra considerably easier than the fit for type II. The number of equivalent sites for each of the inequivalent set is also shown in Table I. Corresponding to these inequivalent sets, we are able to find the exact same number of fine lines for each shell up to $m = 23$ in the P-Al spectrum of 3C-SiC.[8] By comparing with the N-B spectrum,[6] we give the splitting energy for a given shell in Table I. It is found that this splitting energy is almost the same for both N-B and P-Al spectra (e.g., $m = 7$). The exceptions found from $m = 11$ to 17 are probably due to unresolved lines and questionable assignment of shell numbers in this region of the N-B spectrum. Hence, using Eq. (2) we try to fit the P-Al data of Ref. 8.

In Table I we give the calculated splittings $\Delta E = 2|V_3|$ for all sets in the shells $m = 3$–23, using an adjustable value of k_3 to fit the observed splittings of the doublets. We found a very convincing fit for the P-Al data by using $k_3 = \pm 2 \times 10^5$ Å^4 meV from $m = 17$ to 23, as seen in Fig. 2. The calculated values also agree very well with the experimental N-B data from $m = 18$ to 21, as shown in Table I. The sign of k_3 remains undetermined for type-I spectra, but its value is close to that obtained in GaP ($k_3 = \pm 2.4 \times 10^5$ Å^4 meV).[13] Beyond $m = 23$ the substructure of the shells in the P-Al spectrum is no longer

TABLE II. Comparison of the calculated splittings of type-II DAP substructures and observed values in 3C-SiC. Shells, inequivalent sets of lattice vector $\langle uvw \rangle$ in units of $\frac{1}{4}a_0$for a given shell, and the number of sites for equivalent sets of the same shell are also shown between $m = 8$ and 17. The calculated splittings ΔE are obtained from the difference of the octupole term V_3 between inequivalent sets within the same shell. The calculation was performed using $k_3 = -2 \times 10^5$ Å^4 meV. Some of the N-Al DAP data are from Ref. 4 and N-Ga DAP data from Ref. 5.

					ΔE (meV) Observed N-Al		ΔE (meV) Observed N-Ga	
Shell m	$\langle uvw \rangle$ ($\frac{1}{4}a_0$)	Number of sites	V_3 (meV)	ΔE (meV) Calculated	S1	Ref. 4	S2	Ref. 5
8	$\langle 731 \rangle$	24	−1.886	8.6	8.3	8.5	8.5	8.9
8	$-\langle 553 \rangle$	12	6.736					
9	$-\langle 733 \rangle$	12	3.625	–	–	–	–	–
10	$\langle 555 \rangle$	4	−4.847	6.2	–	–	–	–
10	$-\langle 751 \rangle$	24	1.357					
11	$\langle 753 \rangle$	24	−2.856	2.6	2.4	2.2	–	2.5
11	$\langle 911 \rangle$	12	−0.245					
12	$-\langle 931 \rangle$	24	0.532	–	–	–	–	–
13	$\langle 933 \rangle$	12	−1.189	3.8	4.3	4.9	–	4.9
13	$\langle 771 \rangle$	12	−0.719					
13	$-\langle 755 \rangle$	12	2.568					
14	$\langle 951 \rangle$	24	−0.503	2.1	2.3	2.5	–	2.0
14	$-\langle 773 \rangle$	12	1.643					
15	$-\langle 953 \rangle$	24	1.173	–	–	–	–	–
16	$\langle 775 \rangle$	12	−1.682	1.7	1.6	1.7	–	1.8
16	$-\langle 11,1,1 \rangle$	12	0.075					
17	$\langle 955 \rangle$	12	−1.239	1.6	2.1	2.2	–	1.8
17	$\langle 11,3,1 \rangle$	24	−0.182					
17	$-\langle 971 \rangle$	24	0.347					

distinguishable because of the merging of neighboring shell lines. As seen in Table I, the calculated values fail to fit the data for small m ($m < 17$). This failure is probably due to our omission of the *initial* interaction between the neutral donor and acceptor before recombination. The van der Waals term E_{vdW} used in early work to correct line positions of close pairs has no directional dependence, and the experimental data for close pairs strongly deviates from the R^{-6} dependence.[12] At present, there is no possibility to fit the data by further consideration of multipole terms for the initial state without a theory which accounts for the deformation of the donor-electron and acceptor-hole wave functions when the donor and the acceptor are closely spaced. Also, for very close pairs the multipole term alone may not be sufficient to adjust the Coulomb interaction between the ionized donor and acceptor in the final state, as suggested by Patrick.[13]

Since the term V_4 does not give any contribution to splitting into doublets for type-I spectra, we consider now the splitting in type-II DAP spectra to obtain information about k_4.

B. Type II spectra

The most interesting observation is that, by comparing splittings for a given shell in our N-Al and N-Ga DAP substructures with higher-resolution N-Al data from Choyke and Patrick[4] and N-Ga data from Kuwabara *et al.*,[5] we find that the splitting energy for a given shell is almost independent of the identity of the acceptor for all these type-II DAP spectra in 3C-SiC, as seen in Table II and Fig. 1. This suggests that the multipole interaction of the final state between N and Al ions is similar to that between N and Ga ions.

In Table II, we also list shells, inequivalent sets, and the number of sites for each set within the same shell from $m = 8$ to 17. Type-II sets give either positive or negative sign due to the lack of inversion center. To analyze the shell line splitting we follow the procedure used for GaP spectra by adjusting the values of k_3 and k_4. Starting from the parameter values $k_3 = -2.4 \times 10^5$ Å^4 meV and $k_4 = 1.9 \times 10^6$ Å^5 meV which are directly extracted from the literature data on GaP,[14] we find predicted results very far from the experimental values. To improve the agreement, one has to adjust the two parameters independently. Since we have obtained a good fit for N-B and P-Al spectra and got a reasonable value for k_3, we fixed $k_3 = -2 \times 10^5$ Å^4 meV and changed the value of k_4 only. In order to obtain a good fit, we have to reduce k_4 by at least one order of magnitude ($\sim 10^5$ Å^5 meV), which results in a negligible value for V_4. This suggests that the splitting of discrete N-Al and N-Ga DAP lines in 3C-SiC is mainly determined by the octupole component V_3.

Indeed, considering V_3 alone and using $k_3 = -2 \times 10^5$ Å^4 meV, we find that the calculated values agree very well with the observed splitting values between $m = 8$ and 17, as seen in Table II. This is also illustrated in Fig. 3, which includes

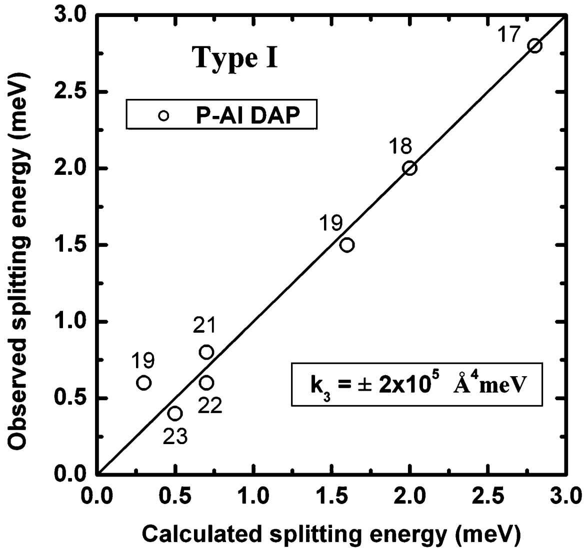

FIG. 2. Comparison of observed and calculated splitting energy (the value from Table I) for discrete lines between $m = 17$ and 23. The calculation was performed using $k_3 = \pm 2 \times 10^5$ Å^4 meV. The P-Al DAP data are from Ref. 8.

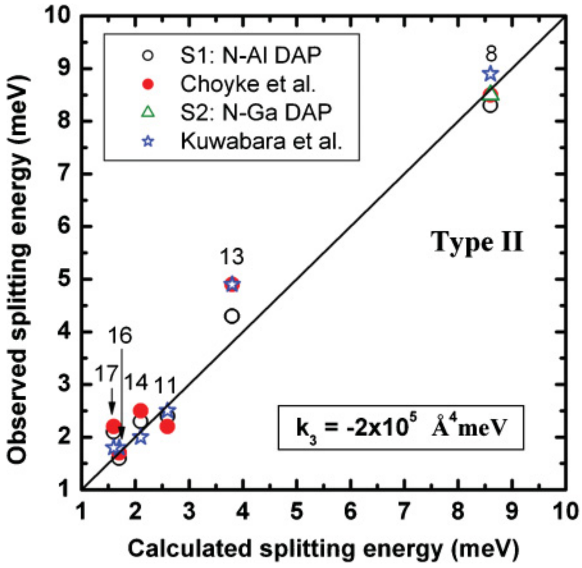

FIG. 3. (Color online) Comparison of observed and calculated splitting energy (the value from Table II) for discrete lines between $m = 8$ and 17. The calculation was performed using $k_3 = -2 \times 10^5$ Å^4 meV. The N-Al DAP data are from Choyke and Patrick(Ref. 4) and N-Ga DAP data from Kuwabara *et al.* (Ref. 5).

all the data from Table II, as well. It should be noted that all the components for each shell in the region of $8 \leqslant m \leqslant 17$ can be clearly resolved (with the above-mentioned exception of $m = 10$) in all available N-Al and N-Ga spectra. For the larger shell numbers $m > 17$ in our N-Al spectra, the splittings become too small for the substructure to be well resolved, as seen in Fig. 1.

Thus we conclude that for both type-I and type-II DAP spectra in 3C-SiC, involving either N or P as donor and Al, Ga, or B as acceptor, the splitting energy of the shell substructure can be successfully explained by the octupole term V_3 alone, with $k_3 = -2 \times 10^5$ Å^4 meV.

To explain this observation, we must consider the delocalization of the ion charge for both the donor and the acceptor. For donors in 3C-SiC, the experimental binding energy of N is 54.2 meV (Ref. 2) and 48.1 meV for P.[8] These values are very close to the 47.2 meV calculated by effective-mass model for a donor with no chemical shift.[16,17]

The effective-mass theory (EMT) is based on the assumption of Coulomb attraction between the electron (hole) and the donor (acceptor) core as point charge, and does not include any information concerning the multipole terms describing the real donor (acceptor) charge distribution. Indeed, if the ground state of a donor (acceptor) can be accurately calculated using the EMT, the deviation of the experimental donor (acceptor) binding energy from the ground state of the EMT value is a sign of the deviation of the core potential from that of a point charge which, however, conforms to the crystal symmetry, and therefore can be accounted for by suitable choice of the multipole terms in the DAP recombination. Thus, the proximity of the binding energies of N and P to the effective-mass value indicates that both N and P ionic charges can be approximately treated as point charges without contribution from multipole terms, leading to negligible values of both k_3 and k_4. On the other hand, all the acceptors are much deeper than the donors and seem to exhibit also large chemical shifts. By using the presently accepted value of 27 meV for the free exciton binding energy in 3C-SiC,[2] the experimental acceptor binding energies are 270, 359, and 749 meV for Al, Ga, and B, respectively. These values are much larger than what would be calculated using the EMT with Coulomb interaction between point charges only. An estimation using the EMT in the spherical approximation of Baldereschi and Lipari[18] yields a value of ∼61 meV for the acceptor binding energy in 3C-SiC within the infinite spin-orbit-coupling limit and a value of ∼67 meV in the case of zero spin-orbit coupling.[19] This shows that the experimental acceptor ground-state energies (Al,Ga,B) in 3C-SiC are subject to large chemical shifts, indicating large deviations of the central-cell ion potential from that of a point charge. Hence, it is reasonable to believe that the acceptor-ion charge distributions are significantly distorted in accord with the T_d point group symmetry. We are led to conclude that the main contribution to the obtained value of k_3 is due to the deviations of the acceptor-ion cores for Al, Ga, and B from point charges, although at this moment we cannot provide a further detailed explanation of why the splitting energy for a given shell is well described by the same value of k_3 for different acceptors.

Coming back to the coefficient k_4, we notice that in GaP, the splitting energy of the given shell substructure of the O-Zn spectrum is different from that in the spectrum of O-Cd.[14,15] This difference is accounted for by changing the k_4 value from 1.9×10^6 to 2.8×10^6 Å^5 meV while keeping $k_3 = -2.4 \times 10^5$ Å^4 meV fixed. In GaP, the O donor is very deep (895 meV) and the acceptors shallow (48,64,96.5 meV for C,Zn,Cd, respectively).[15] Thus, the splittings in GaP are explained by the assumption that k_3 should be attributed to the deep donor. At the same time, the different values found for k_4 were thought to come from the differences in the shallow acceptors. In 3C-SiC, the situation is just the opposite. The donors are very shallow but all the acceptors are much deeper. Compared with GaP, another difference is that for a given shell, the splitting energy is almost independent of acceptor species for both type-I and type-II spectra, as mentioned above. That is why we attributed k_3 to acceptors and believe that k_4 is associated with the shallow donors in 3C-SiC. Since both N and P donors can be treated as point charges to a very good approximation, their contribution to the values of both k_3 and k_4 is negligible.

IV. CONCLUSION

The discrete series of DAP spectra for both type-I (N-B, P-Al) and type-II (N-Al, N-Ga) recombination lines in 3C-SiC have been investigated and compared by considering the multipole fields of the donor and the acceptor ions. It has been found that the splitting energy is almost independent of the acceptor species (Al,Ga,B) but only depends on the type of DAP spectrum and, for both type I and type II, the amount of splitting can be successfully explained by the octupole term V_3 alone, with $k_3 = -2 \times 10^5$ Å^4 meV. To explain this result, we compare the experimental donor and acceptor binding energies with the values calculated from the effective-mass model and suggest that all shallow donor ions can be treated as point charges while only acceptor-ion charge distributions are distorted, resulting in the experimental value for k_3.

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