PHYSICAL REVIEW B VOLUME 50, NUMBER 16 15 OCTOBER 1994-II

Electronic structure of the $\mathrm{Sb_{Ga}}$ heteroantisite defect in GaAs:Sb

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(Received 19 August 1993; revised manuscript received 25 March 1994)

The defect theory of Hjalmarson *et al.* [Phys. Rev. Lett. **44**, 810 (1980)] combined with the bond-orbital model of Baranowski [J. Phys. C **17**, 6287 (1984)] are used to calculate the wave function and hyperfine-interaction tensor of the $\mathrm{Sb_{Ga}}$ heteroantisite defect in GaAs. The defect potential is extended to the nearest-neighbor sites. The hyperfine-interaction constants are in good agreement with the electron paramagnetic resonance data. The results show that the outward relaxation of nearest-neighbor atoms must be taken into account for the quantitative description of this defect.

I. INTRODUCTION

The existence of the $\mathrm{Sb_{Ga}}$ heteroantisite defect in GaAs has been proven, even though its metastable configuration is still under investigation. The experimental evidence for this defect comes from electron paramagnetic resonance (EPR),[1] photo-EPR,[2] magnetic circular dichroism data,[3] the space-charge technique,[4] and the Hall effect,[5] as well as from deep-level transient spectroscopy (DLTS).[6] All of these data have provided detailed information about the electronic structure of this defect.

In particular, the hyperfine-(hf) coupling constant between the magnetic moment of the unpaired defect electron and the magnetic moment of the antimony nucleus, obtained from the EPR (Ref. 1) and photo-EPR (Ref. 2) experiments is one of the key parameters for understanding the microscopic structure of the heteroantisite defect. From the theoretical standpoint, to calculate this quantity would be interesting. The EPR spectrum from Ref. 1 reveals that the defect is so localized that its EPR spectrum contains little information about the defect's surrounding. Therefore it is an isolated antisite defect $\mathrm{Sb_{Ga}As_4}$. It is supposed that the orbital part of its ground-state wave function is *s*-like This fact indicates that adopting the tight-binding picture may well account for some of the electronic properties.

In the present paper, the theory of the EPR of deep impurity states developed by Ren *et al.*[7] based on the tight-binding theory of defects by Hjalmorson *et al.*[8] is used to calculate the wave function of an electron localized on the $\mathrm{Sb_{Ga}}$ defect in GaAs. To improve the calculated wave function, the defect potential is extended to the nearest-neighbor sites. The amount of lattice relaxation for the nearest-neighbor atoms is evaluated by use of the bond-orbital model of Baranowski.[9] From the calculated wave functions, the hf constants of an electron with an Sb or an As nucleus are obtained and compared with EPR data. In addition, the influence of lattice relaxation on the wave function and thereby on the hf constant is discussed. It is found that our results are comparable with those of calculations based on density-functional theory (DFT).[10]

The remaining part of this paper is organized as follows. Section II describes the method used for the present calculation. The results will be presented in Sec. III, followed by a discussion of their meaning and comparison with the available experiments and theory. A brief summary is contained in Sec. IV.

II. THEORETICAL FORMALISM

A. Tight-binding Green-function method

It is recognized that the electronic properties of localized defects in solids can be adequately described using the Koster-Slater tight-binding Green-function technique.[11] The defect electron state $|\psi\rangle$ bound by the short-range potential V satisfies the Schrödinger equation

$$(H_0+V)\psi=E\psi\ , \tag{1}$$

where E is the defect electron energy. In terms of the Green function $[G_0(E)=(E-H_0)^{-1}]$ of the host crystal, the above equation can be written as

$$\psi=G_0(E)V\psi \tag{2}$$

or

$$[I-G_0(E)V]\psi=0\ . \tag{3}$$

The bound-state energies E of the defect satisfy the determinantal equation

$$\det[I-G_0(E)V]=0\ . \tag{4}$$

The wave function ψ has a nontrivial solution. If the perturbation matrix V is nonzero only in a very small subspace of the full Hilbert space H_0, the problem can be treated efficiently in a basis of localized functions.

The EPR spectra of the $\mathrm{Sb_{Ga}}$ antisite defect in GaAs show that the antisite antimony atom is surrounded by a tetrahedron of four equivalent arsenic atoms and is in an

s-like state, with the breathing-mode relaxation. From group theory, the defect state $|\psi\rangle$ transforms according to the irreducible representation A_1 of the T_d point group. Hence $|\psi\rangle$ is expanded in a set of basis functions $|A_1Rm\rangle$,

$$|\psi\rangle=\sum_{Rm}|A_1Rm\rangle\langle A_1Rm|\psi\rangle \ , \tag{5}$$

where $|A_1Rm\rangle$ are orthogonal symmetric combinations of sp^3 hybrid orbitals around the antisite atom. R indexes the Rth shell around the antisite atom site, e.g., $R=0$ for the antisite atom and $R=1$ for the shell of the nearest neighbors, and m marks the mth basis function of the Rth shell transforming according to the A_1 irreducible representation. For example, the s orbital of the antisite antimony atom forms the basis function $|A_101\rangle=|S\rangle$. The A_1 combination of four inward-directed hybrids centered at the nearest-neighbor sites constructs $|A_111\rangle$, and so on.

In the present study, both the diagonal matrix elements of V on the nearest neighbors of the antisite atom and the off-diagonal matrix elements of V, which couple the antisite atom to its nearest neighbors, are included. Thus the potential parameters being introduced are the following:

$$V_{00}=\langle A_101|V|A_101\rangle=\langle S|V|S\rangle \ ,$$

$V_{01}=\langle A_101|V|A_111\rangle$, $V_{10}=\langle A_111|V|A_101\rangle$, and $V_{11}=\langle A_111|V|A_111\rangle$. Then the solution of Eq. (2) reduces to

$$\begin{aligned}\langle A_1Rm|\psi\rangle=&\langle A_1Rm|G|A_101\rangle V_{00}\langle A_101|\psi\rangle\\&+\langle A_1Rm|G|A_101\rangle V_{01}\langle A_111|\psi\rangle\\&+\langle A_1Rm|G|A_111\rangle V_{10}\langle A_101|\psi\rangle\\&+\langle A_1Rm|G|A_111\rangle V_{11}\langle A_111|\psi\rangle \ ,\end{aligned} \tag{6}$$

in which the Green-function matrix elements of the host crystal can be obtained from

$$\langle A_1Rm|G|A_1R'm'\rangle=\sum_{n\mathbf{k}}\frac{\langle A_1Rm|n\mathbf{k}\rangle\langle n\mathbf{k}|A_1R'm'\rangle}{E-E_{n\mathbf{k}}} \ . \tag{7}$$

Here $E_{n\mathbf{k}}$ and $|n\mathbf{k}\rangle$ are the eigenvalues and eigenvectors of the host Hamiltonian which is described by an empirical tight-binding Hamiltonian H_0,[12] and the summation on wave vector $\mathbf{k}$ in the Brillouin zone is performed with use of the special $\mathbf{k}$-point method of Chadi and Cohen.[13]

Because the defect potential V only extends up to the atoms of the $R=1$ shell, a set of linear homogeneous equations for $\langle A_101|\psi\rangle$ and $\langle A_111|\psi\rangle$ may be obtained from Eq. (6):

$$\begin{aligned}\langle A_101|\psi\rangle=&(G_{00}V_{00}+G_{01}V_{10})\langle A_101|\psi\rangle\\&+(G_{00}V_{01}+G_{01}V_{11})\langle A_111|\psi\rangle \ ,\\\langle A_111|\psi\rangle=&(G_{10}V_{00}+G_{11}V_{10})\langle A_101|\psi\rangle\\&+(G_{10}V_{01}+G_{11}V_{11})\langle A_111|\psi\rangle \ ,\end{aligned} \tag{8}$$

where G_{ij} is the abbreviation of the Green-function matrix elements, i.e., $G_{00}=\langle A_101|G|A_101\rangle$, $G_{01}=\langle A_101|G|A_111\rangle$, $G_{10}=\langle A_111|G|A_101\rangle$, and $G_{11}=\langle A_111|G|A_111\rangle$. The determinantal equation (4) reduces to

$$\begin{vmatrix}G_{00}V_{00}+G_{01}V_{10}-1 & G_{00}V_{01}+G_{01}V_{11}\\ G_{10}V_{00}+G_{11}V_{10} & G_{10}V_{01}+G_{11}V_{11}-1\end{vmatrix}=0 \ . \tag{9}$$

Because of the restriction of Eq. (9), only one of the two equations in (8) is independent. The normalization condition $\langle\psi|\psi\rangle=1$ gives another independent equation for $\langle A_101|\psi\rangle$ or $\langle A_111|\psi\rangle$:

$$\begin{aligned}-(C_1+C_3)^2\frac{dG_{00}}{dE}-(C_2+C_4)^2\frac{dG_{11}}{dE}&\\-2(C_1+C_3)(C_2+C_4)\frac{dG_{01}}{dE}&=1 \ ,\end{aligned} \tag{10}$$

where $C_1=V_{00}\langle A_101|\psi\rangle$, $C_2=V_{10}\langle A_101|\psi\rangle$, $C_3=V_{01}\langle A_111|\psi\rangle$, and $C_4=V_{11}\langle A_111|\psi\rangle$.

If the matrix elements of the defect potential are known, the combination of one of the two equations in (8) with Eq. (10) gives the wave functions $\langle A_101|\psi\rangle$ and $\langle A_111|\psi\rangle$. Then the $\langle A_1Rm|\psi\rangle$ for each shell can be obtained from Eq. (6).

B. Defect potential

An adequate representation of the effective impurity potential needed to define the defect as a deep trap requires precise understanding of effects such as Coulomb interactions, lattice relaxation, and charge-state splitting. In the tight-binding method, one can avoid some of these effects by making use of the trends of the perfect-crystal Hamiltonian matrix elements and by defining the perturbation V in a qualitative way.

With regard to the matrix elements of V, the diagonal element V_{00} used is the same as given by Hjalmarson *et al.*[8] for the strain-free theory,

$$V_{00}=\beta_s[\omega_s(\mathrm{Sb})-\omega_s(\mathrm{Ga})] \ , \tag{11}$$

where $\omega_s(\mathrm{Sb})$ and $\omega_s(\mathrm{Ga})$ are the s-orbital atomic energies for the antisite atom Sb and host atom Ga, respectively. Following Ref. 14, and for the same reason, $\beta_s=1$ is used here.

The off-diagonal matrix elements are written as

$$V_{01}=V_{10}=W[(d)^{-2}-(d_0)^{-2}] \ , \tag{12}$$

where W is a proportionality constant, which can be obtained from the parameters of Harrison,[15] and d and d_0 are the bond lengths of the antisite- (impurity-) containing crystal and the perfect crystal, respectively.

It can be imagined that the diagonal matrix elements of the defect potential at the nearest-neighbor sites, V_{11}, should be dependent on d/d_0. Under the condition of absence of relationship between V_{11} and d/d_0, the direct calculation of V_{11} is difficult. However, fortunately, Eq. (9) can be used to determine the relationship if the energy level E and lattice relaxation d are fixed.

C. Local lattice relaxation

In order to determine $V_{01}(V_{01})$, the local bond length between the antisite atom and its nearest neighbors must be defined first. An approximate estimation of the impurity-host relaxation in semiconductors has been suggested by Baranowski.[9] In the notation of Harrison,[15] the gain in the impurity-host bond energy per bond connected with a distortion Δd ($\Delta d > 0$ outward and $\Delta d < 0$ inward) can be calculated as

$$\Delta E_b = \Delta E_b^1 + \Delta E_b^2 \ , \tag{13a}$$

where ΔE_b^1 and ΔE_b^2 are, respectively, the changes in the energy of the bonds caused by distortion in the nearest-neighbor and second-nearest-neighbor atom positions. These are given by

$$\begin{aligned}\Delta E_b^1 = -2\{ & [V_2^2(d_0+\Delta d)+V_3^2]^{1/2} - V_2^2(d_0+\Delta d)/k|\bar{\varepsilon}_h| \\ & -[V_2^2(d_0)+V_3^2]^{1/2} + V_2^2(d_0)/k|\bar{\varepsilon}_h|\} \ ,\end{aligned} \tag{13b}$$

and

$$\begin{aligned}\Delta E_b^2 = -6\{ & [V_2'^2(d_0+\Delta d')+V_3'^2]^{1/2} \\ & - V_2'^2(d_0+\Delta d')/k'|\bar{\varepsilon}_h'| \\ & -[V_2'^2(d_0)+V_3'^2]^{1/2} + V_2'^2(d_0)/k'|\bar{\varepsilon}_h'|\} \ ,\end{aligned} \tag{13c}$$

in which V_2 ($\equiv \zeta d^{-2}$), V_3, and $k|\bar{\varepsilon}_h|$ refer to the covalent and polar bond energies and the average hybrid energy of the impurity nearest-neighbor bond, respectively; they are dependent on the charge state of the defect. The terms V_2', V_3', and $k'|\bar{\varepsilon}_h']$ are the covalent and polar bond energies and average hybrid energy of the host crystal (see Ref. 9 for further details). $\Delta d'$ is the change in bond length between the first and second nearest neighbors. If the second nearest neighbors are held fixed, then the following formula is derived:

$$\Delta d' = [d_0^2 - \tfrac{2}{3} d_0 \Delta d + (\Delta d)^2]^{1/2} - d_0 \ . \tag{13d}$$

Within this approximation, the minimum of the total energy predicts the impurity-host relaxation, i.e., gives the local bond length d.

D. Hyperfine-interaction tensor

In order to use the symmetric wave function $\langle A_1 Rm|\psi\rangle$ to calculate the hf-interaction tensor, we now expand the electronic state $|\psi\rangle$ in terms of the atomic orbitals

$$|\psi\rangle = \sum_j [C_{jS}|jS\rangle + C_{jX}|jX\rangle + C_{jY}|jY\rangle + C_{jZ}|jZ\rangle] \ , \tag{14}$$

where $|jS\rangle$, $|jX\rangle$, $|jY\rangle$, and $|jZ\rangle$ are the nS and nP atomic orbitals of the host or antisite at the jth site, respectively. $C_{jS} = \langle jS|\psi\rangle$, $C_{jX} = \langle jp_X|\psi\rangle$, $C_{jY} = \langle jp_Y|\psi\rangle$, and $C_{jZ} = \langle jp_Z|\psi\rangle$ can be evaluated using the calculated $\langle A_1 Rm|\psi\rangle$.

As usual, the probability of the unpaired electron on the jth atom is represented by

$$\eta_j^2 = C_{jS}^2 + C_{jX}^2 + C_{jY}^2 + C_{jZ}^2 \tag{15}$$

and the percentage s and p character of the wave function by

$$\begin{aligned} &\alpha_j^2 = C_{jS}^2/\eta_j^2 \ , \\ &\beta_j^2 = (C_{jX}^2 + C_{jY}^2 + C_{jZ}^2)/\eta_j^2 \ , \\ &\alpha_j^2 + \beta_j^2 = 1 \ . \end{aligned} \tag{16}$$

The principal values of the hyperfine-interaction tensor can be parametrized as

$$\begin{aligned} &(A_{\parallel})_j = a_j + 2b_j \ , \\ &(A_{\perp})_j = a_j - b_j \ , \end{aligned} \tag{17}$$

where the hf-interaction parameters a_j represent the isotropic part of the hf interaction, and b_j gives the purely axially symmetric part of the hf interaction. They are given by

$$\begin{aligned} &a_j = \alpha_j^2 \eta_j^2 A_{jf} \ , \\ &b_j = \beta_j^2 \eta_j^2 B_{jf} \ , \end{aligned} \tag{18}$$

with

$$\begin{aligned} &A_{jf} = (16\pi/3)(\mu_j/I_j)\mu_B|\psi_{nS}(0)|_j^2 \ , \\ &B_{jf} = \tfrac{4}{5}(\mu_j/I_j)\mu_B\langle r_{nP}^{-3}\rangle_j \end{aligned} \tag{19}$$

in which μ_B is the Bohr magneton, and μ_j and I_j are the nuclear magneton and nuclear spin of the jth atom, respectively. $|\psi_{nS}(0)|_j^2$ and $\langle r_{nP}^{-3}\rangle_j$ are the probability density of the *ns* orbital of the jth atom at its nucleus site and the expectation value of r^{-3} weighted over the *np* orbital of the jth atom, respectively. For ^{75}As, the natural abundance is 100%, $I=\frac{3}{2}$, $\mu = 1.439$ nm, $|\psi_{4S}(0)|^2 = 93.9\times 10^{24}$ cm^{-3}, and $\langle r_{4P}^{-3}\rangle = 49.4\times 10^{24}$ cm^{-3}. Antimony has two isotopes ^{121}Sb and ^{123}Sb with natural abundances of 57% and 43%, respectively. The nuclear spins are $I_{121} = \frac{5}{2}$ and $I_{123} = \frac{7}{2}$, and the nuclear magnetons are $\mu_{121} = 3.3593$ nm and $\mu_{123} = 2.5465$ nm, respectively. $|\psi_{5S}(0)|^2 = 148.1\times 10^{24}$ cm^{-3} and $\langle r_{5P}^{-3}\rangle = 82.3\times 10^{24}$ cm^{-3} are the same for ^{121}Sb and ^{123}Sb. These values are taken from Ref. 16.

The relationship of the effective value of the hf interaction constant A_{eff} with the direction of the externally applied magnetic field is given by

$$A_{\text{eff}} = (A_1^2 n_1^2 + A_2^2 n_2^2 + A_3^2 n_3^2)^{1/2} \ , \tag{20}$$

where A_1, A_2, and A_3 are the principal values of the hf tensor $\mathbf{A}$ and n_1, n_2, and n_3 are the direction cosines of the magnetic field direction with respect to the 1, 2, and 3 principal axes of the $\mathbf{A}$ tensor.

III. RESULTS AND DISCUSSION

A group-V atom on a group-III site in a III-V compound, i.e., an anion antisite defect, should act as a double donor. A double donor can exist in three charge states, D^0, D^+, and D^{2+}, and may consequently introduce two energy levels in the gap. The energy levels of the $\mathrm{As_{Ga}}$ homoantisite defect are located at $E_C-0.74$ eV $(0/+)$ and $E_V+0.52$ eV $(+/2+)$.[17] The energy-level structure of the $\mathrm{Sb_{Ga}}$ heteroantisite defect in GaAs was found to be consistent with that of a double donor with the $(0/+)$ energy level located at $E_C-0.5$ eV and the $(+/2+)$ energy level located at $E_C-0.7$ eV.[4] It is interesting to note that the energy difference between the first and the second ionization levels is very similar for $\mathrm{As_{Ga}}$ and $\mathrm{Sb_{Ga}}$ in GaAs. Only the one-electron state D^+ is paramagnetic, and the unpaired defect electron of $\mathrm{As_{Ga}}$ in GaAs occupies the $(+/2+)$ energy level, so the unpaired defect electron of $\mathrm{Sb_{Ga}}$ in GaAs occupies the $(+/2+)$ energy level, i.e., $E=E_C-0.7$ eV.

Equations (13a)–(13d) allow us to calculate the local relaxation around various impurities in all semiconductors using the periodic table with values of the atomic terms ε_S and ε_P.[18] The results for the lattice relaxation in GaAs:$\mathrm{Sb_{Ga}}$ obtained at the minima of total energy are shown in Fig. 1. The outward relaxations of nearest-neighbor atoms for D^0, D^+ charge states are determined to be 7.0% and 17.3% of the bond length ($d_0=2.45$ Å, $\Delta d=0.17$ and 0.42 Å), respectively. Our results are comparable to the DFT result for the neutral heteroantisite $\mathrm{Sb_{Ga}}$ in GaAs, $\Delta d=0.27$ Å, obtained by Caldas *et al.*[10] Using the experimental value of the defect energy level E $(=E_C-0.7$ eV$)$ and the theoretical value of the lattice relaxation d/d_0 $(=1.173)$, the combination of Eqs. (11) and (12) with Eq. (9) gives the V_{11} $(=-2.567$ eV$)$.

In order to investigate the effect of lattice relaxation on defect energy level, we assume that V_{11} will vary as a function of lattice relaxation and $V_{11}=0$ when $d=d_0$. The simplest assumption is that $V_{11}=k(d/d_0-1)$.[19] According to the obtained values of d/d_0 $(=1.173)$ and V_{11} $(=-2.567$ eV$)$, the parameter k $(=-14.8)$ is obtained. Then the trends of defect energy level, electronic wave functions, and hf-interaction constants with relative lattice relaxation d/d_0 can be explored.

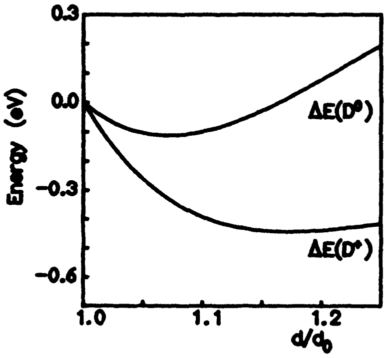

FIG. 1. Calculated lattice distortion in GaAs:$\mathrm{Sb_{Ga}}$ based on bond-orbital model. The total $(\Delta E=\Delta E_1+\Delta E_2)$ bond-energy variation is plotted against $\Delta d/d_0$ for a single heteroantisite defect. The minimum of the total energy predicts the relaxation of the nearest-neighbor lattice. The outward relaxations of nearest-neighbor atoms for D^0, D^+ charge states are determined to be 7.0% and 17.3% of the bond length.

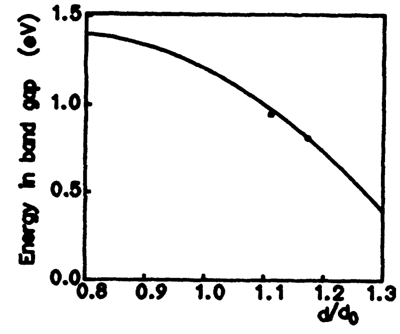

FIG. 2. The dependence of the deep energy level of the $\mathrm{Sb_{Ga}}$ heteroantisite in GaAs on lattice relaxation. The dot indicates $E=E_C-0.70$ eV (Ref. 4) and $d/d_0=1.173$. The black square indicates $E=E_V+0.95$ eV and $d=d_0+0.27$ Å (Ref. 10), i.e., $d/d_0=1.10$. The line is the theoretical curve.

The trend of the A_1 level vs the lattice relaxation obtained from Eq. (9) is shown in Fig. 2. This curve indicates that the energy level moves closer to the conduction-band edge for inward relaxation from the center, while it moves deeper into the band gap for outward relaxation. We note that a similar trend has been predicted for various Ga-site and P-site impurities in GaP and S, Se, and Te in Si by Li and Myles,[20] for N in GaP by Shen, Ren, and Dow[14] and for $\mathrm{P_{Ga}}$, $\mathrm{As_{Ga}}$, and $\mathrm{Sb_{Ga}}$ in GaAs by Caldas *et al.*[10] It is clear from Fig. 2 that, when $d/d_0=1.07$, the energy level is located at $E_V+1.07$ eV, i.e., $E=E_C-0.44$ eV; these are approximately equal to the experimental values of 0.48 (Refs. 2,5) and 0.50 eV (Ref. 4) below the conduction-band edge for the $0/+$ energy level. When $d/d_0=1.1$, i.e., $\Delta d=0.27$ Å, the energy level is located at $E_V+1.0$ eV, which approximately equals $E_V+0.95$ eV obtained by Caldas *et al.*[10] for the neutral defect $\mathrm{Sb_{Ga}}$ in GaAs. So the above assumption $V_{11}=k(d/d_0-1)$ is not too crude to describe the relationship between defect energy level and lattice relaxation.

The obtained defect electronic wave functions and the hf-interaction constants are shown in Table I, and compared with the experimental data. From Table I, it can be seen that the probability of an unpaired electron on

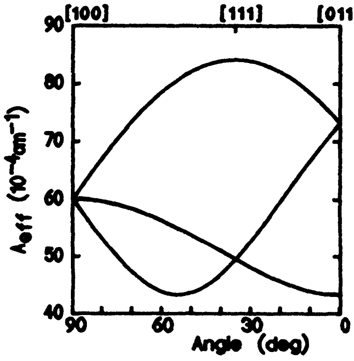

FIG. 3. Angular dependence for the hf-interaction tensors $\mathrm{As_4}$ of the $\mathrm{Sb_{Ga}}$ heteroantisite in GaAs. The magnetic field is rotated in the $(0\bar{1}1)$ plane.

TABLE I. The probabilities η^2 of the unpaired electron, the s-character percentage α^2 and p-character percentage β^2 of the wave functions on the antisite antimony, and the nearest-neighbor arsenic atom in GaAs, and the principal values of hf interactions, i.e., $A_{\parallel}$ and $A_{\perp}$, the isotropic part a, and the anisotropic b (in 10^{-4} cm^{-1}). The corresponding experimental results are taken from Refs. 1 and 3.

	$A_{\parallel}$	$A_{\perp}$	a	b	α^2 (%)	β^2 (%)	η^2 (%)	Reference
^{121}Sb		2203		0	100	0		Ref. 1
		2200		0	100	0		Ref. 3
		2259		0	100	0	28.7	This work[a]
		1215		0	100	0	15.5	This work[b]
^{123}Sb		1200		0	100	0		Ref. 1
		1200		0	100	0		Ref. 3
		1223		0	100	0	28.7	This work[a]
		658		0	100	0	15.5	This work[b]
As$_4$	84.2	43.4	57.0	13.6	9.8	90.2	15.3	This work[a]
	126.1	90.7	102.5	11.8	18.3	81.7	14.6	This work[b]

[a] The outward relaxation of the nearest neighbor is 17.3% of the bond-length, and the deep energy level is located at $E_C - 0.7$ eV[4].

[b] The unrelaxed case where the deep energy level is located at $E_V + 1.21$ eV.

the antisite antimony in the relaxed case is larger than in the unrelaxed case. This means that the probability for outward relaxation increases. The probabilities of the unpaired electron on the nearest-neighbor atoms in the relaxed and unrelaxed cases are approximately equal to each other, i.e., the probabilities of the unpaired electron on the four nearest-neighbor arsenic atoms are almost independent of its relaxation. Therefore an increase in the bond length causes an increase in localization of its wave function, which is identical with the result of the density-functional theory calculations for P, As, and Sb in GaAs and InP by Caldas *et al.*[10] The s-character percentage of the wave function on the antisite atom does not change with the bond length variation; however, the s-character percentage of the wave function on the nearest neighbors decreases for outward relaxation.

The calculated hf-interaction constant at the central antimony atom in the unrelaxed case is much smaller than the experimental data, but in the relaxed case it is in good agreement with the EPR data.[1,3] So the effect of the nearest-neighbor lattice relaxation is very important; it must be taken into account for correct quantitative description of the Sb$_{\text{Ga}}$ heteroantisite defect in GaAs.

It is seen from Table I that the probability of the defect wave function on Sb is 28.7% in the relaxed case. This is approximately equal to the paramagnetic electron density [about 26% (Ref. 21)] at the central atom of the intrinsic anion antisites in GaP, InP, and GaAs. The total probability of the defect electronic wave function on the four nearest-neighbor As atoms is about 61%; this also approximately equals that of the homoantisite in GaP, InP, and GaAs. That is to say, the wave functions of the anion heteroantisite and homoantisite defects in GaP, InP, and GaAs become more similar after the lattice relaxes in the breathing mode.

The calculated results of the hf-interaction constants with the nearest-neighbor As atoms are also listed in Table I. The angular dependence of the effective A values, A_{eff}, for rotation of the magnetic field in the $(0\bar{1}1)$ plane has been predicted, and is shown in Fig. 3. It reveals the characteristic four-line (two of them are coincident) spectrum of the four As$_4$ units, each with a different [111] axis of symmetry. The results may be useful for future interpretation of electronic structure detected in experiments.

IV. SUMMARY

The theory of the EPR spectrum of deep impurity states combined with the bond-orbital model are used to investigate the electronic structure of the heteroantisite defect Sb$_{\text{Ga}}$ in GaAs. Using the bond-orbital model, the outward relaxation of the nearest-neighbor lattice is determined. The result shows that the relaxation must be taken into account for the quantitative description of the Sb$_{\text{Ga}}$ heteroantisite defect in GaAs. The calculated defect electronic wave functions show that the wave function of the anion heteroantisite and homoantisite defect in GaP, InP, and GaAs become more similar after the lattice relaxes in the breathing mode, and the calculated hf-interaction constants are in good agreement with the EPR data.

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