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Oscillator strengths of shallow impurity spectra in germanium and silicon

P. Clauws
Laboratorium voor Kristallografie en Studie van de Vaste Stof, Rijksuniversiteit Gent, Krijgslaan 281-S1, B-9000 Gent, Belgium

J. Broeckx
Université du Burundi, Faculté des Sciences, BP 2700, Bujumbura, Republic of Burundi

E. Rotsaert and J. Vennik
Laboratorium voor Kristallografie en Studie van de Vaste Stof, Rijksuniversiteit Gent, Krijgslaan 281-S1, B-9000 Gent, Belgium

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The oscillator strength of dipole transitions of donors in silicon and germanium and of acceptors in germanium is calculated in the effective-mass approximation. A point-charge potential including variable screening allows one to adjust the ground state to the range of experimental binding energies and to explore the effect of the central-cell correction on the oscillator strength. Calculated f values are listed up to $7p_\pm$ for the different group-V donors and up to $9\Gamma_8^-$ for the different group-III acceptors. A comparison with recent experimental oscillator strengths is made. The results are in fair agreement with the experimental data concerning the structure of the spectra and the chemical trend of the absorption cross section. The assignment of the C line and the A multiplet in the spectrum of acceptors in germanium is substantiated.

I. INTRODUCTION

The electronic state spectrum of shallow impurities in silicon and germanium is well known and understood. Detailed absorption spectra have been obtained for a number of defects, among which are the substitutional group-V donors and group-III acceptors; a survey may be found in the review by Ramdas and Rodriguez.[1] Effective-mass calculations for donors[2–5] and acceptors[6,7] have been very successful in giving excited-state energies in close agreement with the experimental data so that the assignment of most absorption lines is well established. Information concerning the absorption cross section of the lines and the oscillator strength of the transitions is, however, limited in comparison with the many data that are available on the structure of the spectra and the level energies. Yet knowledge of the absorption cross sections makes absorption spectroscopy applicable to absolute impurity analysis and calculated oscillator strengths provide clues for line identification.

We have recently achieved a set of calibration experiments in order to dispose of accurate absorption cross sections for the group-V donors and group-III acceptors in germanium.[8] The data are internally consistent in the sense that they show a clear impurity dependence (chemical shift), i.e., a progressive fall of the oscillator strengths with increasing binding energy as may be intuitively expected from the progressive localization of the ground-state wave function. Similar observations were made by Baber[9] concerning single donors and acceptors in silicon and by Moore[10,11] concerning double acceptors in germanium and single acceptors in GaAs.

Calculated oscillator strengths have been published for donors[12,13] and acceptors[13–16] in germanium and for donors[12,17] and acceptors[16] in silicon. It is interesting that the calculations by Kogan *et al.*[12,13] predict for donors an impurity dependence similar to the experimental observations; the calculated impurity effect for acceptors[15] is, however, much smaller than observed.

In this paper we present new calculated oscillator strengths obtained from similar effective-mass calculations as were used before to obtain the excited-state energies of donors in Si and Ge and acceptors in Ge.[5,18] In order to generate a chemical shift the point-charge potential now includes a variable screening parameter[19] which allows the ground state to be adjusted to any value in the range of observed binding energies. A detailed comparison will be made with the experimental data and with previous calculations.

II. THEORY

The oscillator strength of an electric dipole transition between effective-mass states a and b may be defined as[20]

$$f_{ab}=\frac{2m^*}{\hbar^2}(E_b-E_a)|\mathbf{1}\cdot\mathbf{r}_{ba}|^2 , \tag{1}$$

with m^* the effective mass, E_b-E_a the energy of the transition, $\mathbf{r}_{ba}$ the dipole matrix element, and $\mathbf{1}$ the unit polarization vector of the radiation. In order to satisfy the sum rule $\sum_b f_{ab}=1$, the correct effective mass must be used. For shallow donors and acceptors in Si and Ge, the harmonic mean

$$m^*=\left[\frac{1}{3}\left[\frac{1}{m_\parallel^*}+\frac{2}{m_\perp^*}\right]\right]^{-1}$$

should be taken.[21] For acceptors in cubic semiconductors the sum rule is governed only by the Luttinger valence band parameter γ_1,[14] i.e., $m^*=m_0/\gamma_1$.

Experimentally the oscillator strength is determined from the integrated absorption cross section of the absorption band corresponding with the transition $a \rightarrow b$,[20]

$$f_{ab} = \left[\frac{nm^*c}{2\pi^2 e^2 \hbar} \right] \left[\frac{\mathcal{E}_0}{\mathcal{E}_{\text{eff}}} \right]^2 \int_{\text{band}} \sigma(\hbar\omega) d(\hbar\omega) , \tag{2}$$

with $\sigma = \alpha / N_{\text{imp}}$ the absorption cross section (α is the absorption coefficient and N_{imp} the density of absorbing centers), n the refractive index of the semiconductor, $\mathcal{E}_0$ the average electric field in the medium, and $\mathcal{E}_{\text{eff}}$ the field effective in inducing the dipole transition. Throughout this paper it will be assumed that the effective field ratio $(\mathcal{E}_0/\mathcal{E}_{\text{eff}})$ equals unity, which according to Dexter[20] should be an excellent approximation for transitions between states with extended wave functions such as effective-mass states in semiconductors.

III. CALCULATED OSCILLATOR STRENGTHS

The eigenfunctions were obtained in the course of effective-mass state calculations similar to those presented in earlier papers on donors in Si and Ge (Ref. 5) and acceptors in Ge.[18] The eigenfunctions are thereby expanded in a truncated series of angular basis functions multiplied by unknown radial functions. Angular matrix elements are evaluated using the reduced matrix element technique[22] and the resulting set of radial differential equations is then solved variationally.[7] A more extensive description can be found in the papers mentioned above.[5,18] For the present calculations the effective-mass Hamiltonian includes a point-charge potential with q-dependent dielectric screening augmented by the phenomenological short-range potential introduced by Lipari *et al.*[19] Expressing energy and length in effective atomic units $R_0^* = m_{\text{eff}} e^4 / 2\hbar^2 \epsilon_\infty^2$ and $a_0^* = \hbar^2 \epsilon_\infty / m_{\text{eff}} e^2$, with ϵ_∞ the static dielectric constant and $m_{\text{eff}} = m_\perp^*$ for donors and $m_{\text{eff}} = m_0 / \gamma_1$ for the acceptors, the total potential is given by

$$-\frac{2}{r}[1 + (\epsilon_\infty - 1)e^{-\alpha' r}] , \tag{3}$$

in which α' is to be regarded as a phenomenological parameter allowing the ground-state energy to adjust to the experimentally observed values.

The oscillator strengths are calculated following (1) for transitions from the ground state. The following material constants were used:[5] for Ge, $m_\perp^* = 0.081\,52 m_0$, $m_\parallel^* = 1.588 m_0$, $\gamma_1 = 13.38$, $\epsilon_\infty = 15.36$; for Si, $m_\perp^* = 0.1905 m_0$, $m_\parallel^* = 0.9163 m_0$, $\epsilon_\infty = 11.40$.

The donor effective-mass calculations correspond to the case of a single conduction band valley. For the transitions from the $1s$ ground state to the odd-parity states with $m = 0$, the oscillator strength is evaluated with the polarization vector parallel to the valley axis and is denoted $f_\parallel$; for transitions to the odd-parity states with $m = \pm 1$ the polarization vector is taken perpendicular to the valley axis yielding $f_\perp$. In order to compare with experimental oscillator strengths it is, however, necessary to take account of the multivalley nature of the conduction band in Si and Ge. The ground-state wave function of the group-V donors may be written as a linear combination of single valley wave functions,

$$\Psi_{1s}(A_1) = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} \phi_{1s,j} , \tag{4}$$

with $N = 4$ for Ge and 6 for Si, so that transitions within each of the valleys contribute to the total oscillator strength.

It is readily shown that for a fixed (but arbitrary) choice of the polarization vector, the oscillator strengths in the multivalley case are as follows, related to the above defined values in the single valley case. For $1s\,(A_1)$ to (n, l = odd, $m = 0$),

$$f_0 = \tfrac{1}{3} f_\parallel ; \tag{5a}$$

for $1s\,(A_1)$ to (n, l = odd, $m = \pm 1$),

$$f_\pm = \tfrac{2}{3} f_\perp . \tag{5b}$$

The symmetry of the acceptor states in germanium within the point-charge approximation is that of $\bar{O}_h$. The ground state is denoted as $1\Gamma_8^+$ and the allowed dipole transitions are towards $n\Gamma_8^-$, $n\Gamma_7^-$, and $n\Gamma_6^-$. The ground state being fourfold degenerate, the oscillator strength is obtained from the oscillator strength of the transitions between the sublevels,

$$f_{1\Gamma_8^+, n\Gamma_g^-} = \tfrac{1}{4} \sum_{i=1}^{4} \sum_{j=1}^{2\text{ or }4} f_{1\Gamma_{8(i)}^+, n\Gamma_{g(j)}^-} , \tag{6}$$

with $g = 6$, 7, or 8. The summation is simplified by choosing the polarization vector along one of the cubic axes.

The screening parameter α' has for each case been adjusted in order to cover the entire range of group-V donors or group-III acceptors. The numerical f values for the individual transitions have been summarized in Tables I–III for ground-state energies coincident with the experimental binding energies. EMA refers to the calculation without variable screening, i.e., the usual effective-mass approximation. The dependence of the oscillator strength on binding energy has been visualized for the main absorption lines in Figs. 1–3. Notice that the donor excited states have been labeled with Faulkner's[3] notation instead of the labeling by Broeckx *et al.*[5] in order to facilitate comparison with previous data on the oscillator strength.

IV. EXPERIMENTAL OSCILLATOR STRENGTHS

Experimental f values to compare with the calculated data given above may be obtained from the cross section of absorption lines using formula (2). Unfortunately only few absolute data seem to be available for silicon. Values for the maximum absorption cross section of the $2p_\pm$ line of phosphorus and arsenic have been published by Baber.[9] Estimates for the integrated cross section $\int \sigma \, d\nu$ (ν is the wave number in cm^{-1}) after multiplication by the linewidth $\Delta\nu = 0.7$ cm^{-1} are then 9.4×10^{-14} cm for P and 5.2×10^{-14} cm for As. The corresponding oscillator strengths are $f_{2p_\pm}(\text{P}) = 0.093$ and $f_{2p_\pm}(\text{As}) = 0.051$.

TABLE I. Shallow donors in silicon: calculated f values of transitions from the 1s ground state. Excited-state labels are according to Faulkner (Ref. 3). Energies are in meV below the conduction band. EMA is the effective-mass approximation.

				Donor		
		EMA	Sb	P	As	Bi
				1s energy		
		31.26	42.74	45.59	53.76	70.98
Excited state	Energy					
$2p_\pm$	6.402	0.2877	0.1520	0.1325	0.0933	0.0502
$3p_\pm$	3.120	0.0549	0.0336	0.0300	0.0225	0.0128
$4p_\pm$	2.187	0.0187	0.0121	0.0108	0.0081	0.0048
$4f_\pm$	1.894	0.0060	0.0040	0.0036	0.0026	0.0016
$5p_\pm$	1.449	0.0149	0.0097	0.0088	0.0064	0.0037
$5f_\pm$	1.260	0.0006	0.0005	0.0005	0.0005	0.0004
$6p_\pm$	1.071	0.0069	0.0042	0.0037	0.0024	0.0012
$6f_\pm$	1.002	0.0000	0.0000	0.0000	0.0001	0.0002
$6h_\pm$	0.886	0.0044	0.0043	0.0043	0.0040	0.0038
$7p_\pm$	0.822	0.0018	0.0008	0.0007	0.0002	0.0000
$2p_0$	11.496	0.0586	0.0350	0.0312	0.0233	0.0135
$3p_0$	5.487	0.0081	0.0069	0.0064	0.0053	0.0035
$4p_0$	3.310	0.0029	0.0027	0.0026	0.0022	0.0015
$4f_0$	2.339	0.0001	0.0001	0.0000	0.0000	0.0000
$5p_0$	2.235	0.0014	0.0014	0.0014	0.0011	0.0009
$5f_0$	1.631	0.0008	0.0008	0.0008	0.0006	0.0005

A list of relative f data may be found in the paper of Bara *et al.*[17]

The situation is better for Ge where the integrated absorption cross section of several lines has been determined by calibration experiments[8,23] using a set of crystals doped with essentially one shallow impurity (i.e., Sb, P, As, B, Al, Ga, or In) and covering the $10^{12}-10^{14}$ atoms/cm^3 range. Experimental details may be found in Refs. 8 and 23. The corresponding f values are summarized in Tables IV and V.

V. DISCUSSION

The calculated f values presented here are in agreement with some of the earlier published results. Our data

TABLE II. Shallow donors in germanium: calculated f values of transitions from the 1s ground state. Excited state labels are according to Faulkner (Ref. 3). Energies are in meV below the conduction band. EMA is the effective-mass approximation. Separate data for Bi are not given since the ground state at 12.75 meV is close to P.

			Donor		
		EMA	Sb	P	As
			1s energy		
		9.84	10.32	12.88	14.18
Excited state	Energy				
$2p_\pm$	1.729	0.2337	0.2099	0.1272	0.1023
$3p_\pm$	1.042	0.0404	0.0375	0.0252	0.0207
$4p_\pm$	0.753	0.0221	0.0207	0.0142	0.0118
$4f_\pm$	0.609	0.0200	0.0184	0.0124	0.0103
$5p_\pm$	0.573	0.0026	0.0025	0.0019	0.0016
$5f_\pm$	0.465	0.0073	0.0070	0.0050	0.0042
$6p_\pm$	0.397	0.0064	0.0060	0.0040	0.0032
$6f_\pm$	0.379	0.0026	0.0024	0.0016	0.0012
$6h_\pm$	0.318	0.0080	0.0075	0.0044	0.0034
$7p_\pm$	0.308	0.0000	0.0000	0.0000	0.0000
$2p_0$	4.776	0.0188	0.0176	0.0125	0.0106
$3p_0$	2.586	0.0020	0.0020	0.0021	0.0020
$4p_0$	1.696	0.0007	0.0007	0.0008	0.0008
$4f_0$	1.220	0.0003	0.0003	0.0004	0.0004

TABLE III. Shallow acceptors in germanium: calculated f values of transitions from the $1\Gamma_8^+$ ground state. Energies are in meV above the valence band. Corresponding line labels of the experimental spectrum are given in column 1.

Line	Excited state	Energy	Acceptor B	 Al	 Ga	 In	 Tl
		$1\Gamma_8^+$ energy	10.81	11.15	11.32	11.99	13.45
G	$1\Gamma_8^-$	4.581	0.0029	0.0025	0.0023	0.0018	0.0009
D	$2\Gamma_8^-$	2.875	0.1007	0.0970	0.0952	0.0884	0.0755
C	$1\Gamma_7^-$	2.125	0.0573	0.0545	0.0531	0.0481	0.0391
C	$3\Gamma_8^-$	2.103	0.0083	0.0078	0.0076	0.0067	0.0051
B	$4\Gamma_8^-$	1.477	0.0054	0.0057	0.0059	0.0063	0.0070
$A4$	$5\Gamma_8^-$	1.210	0.0019	0.0019	0.0020	0.0020	0.0019
$A3$	$1\Gamma_6^-$	1.142	0.0021	0.0020	0.0019	0.0017	0.0013
$A3$	$2\Gamma_7^-$	1.140	0.0037	0.0037	0.0036	0.0035	0.0032
$A3$	$6\Gamma_8^-$	1.128	0.0020	0.0020	0.0019	0.0018	0.0016
$A2$	$3\Gamma_7^-$	1.012	0.0040	0.0038	0.0037	0.0034	0.0028
$A1$	$7\Gamma_8^-$	0.920	0.0025	0.0027	0.0028	0.0031	0.0038
Ii	$8\Gamma_8^-$	0.777	0.0006	0.0007	0.0007	0.0008	0.0011
Ii	$2\Gamma_6^-$	0.756	0.0008	0.0007	0.0007	0.0005	0.0003
Ii	$9\Gamma_8^-$	0.756	0.0004	0.0005	0.0005	0.0005	0.0006

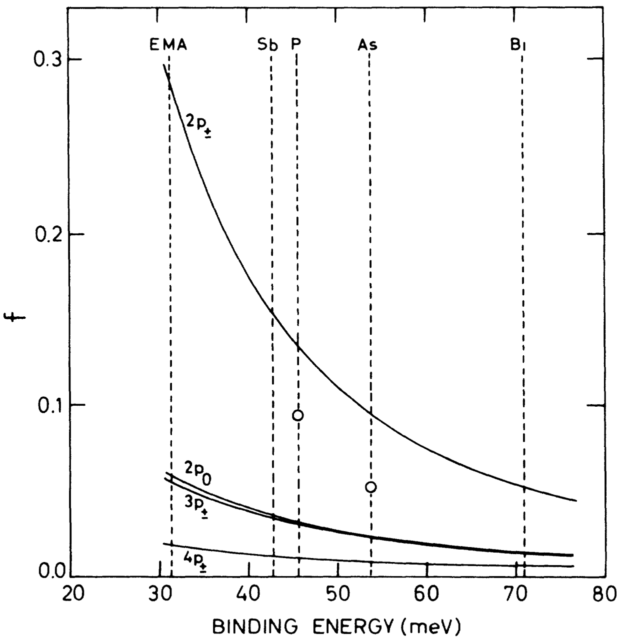

FIG. 1. Donors in silicon: calculated oscillator strength of the main transitions as a function of 1s binding energy (solid lines). The ground-state energy of individual donors is indicated by a vertical line. EMA is the effective-mass approximation. Circles are the experimental $2p_\pm$ data according to Baber (Ref. 9).

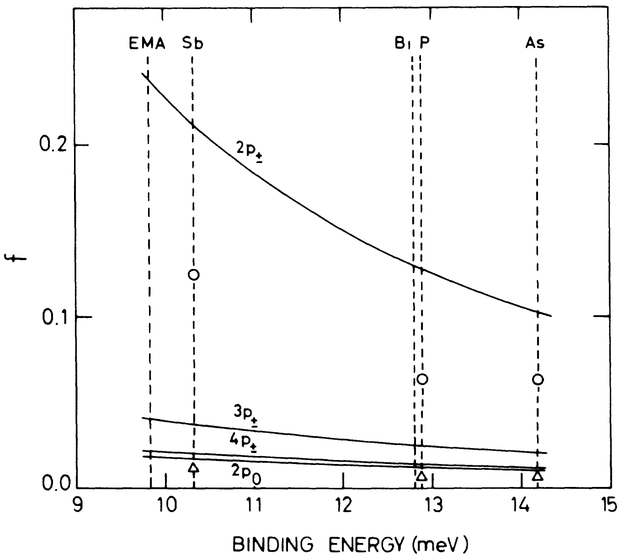

FIG. 2. Donors in germanium: calculated oscillator strength of the main transitions as a function of 1s binding energy (solid lines). The ground-state energy of individual donors is indicated by a vertical line. EMA is the effective-mass approximation. Experimental data according to Rotsaert *et al.* (Refs. 8 and 23): $2p_\pm$ (circles) and $2p_0$ (triangles).

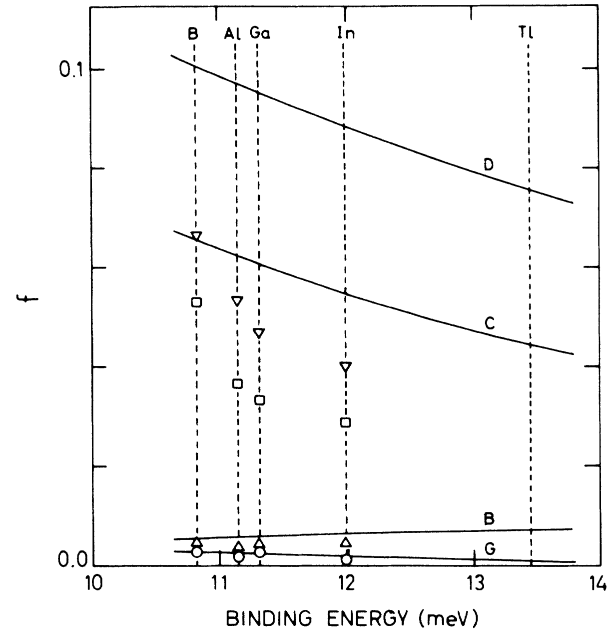

FIG. 3. Acceptors in germanium: calculated oscillator strength of the main transitions as a function of $1\Gamma_8^+$ binding energy (solid lines). The excited states are indicated by their absorption spectrum label (see Table III for the correspondence); the result for the C line is the sum of the contribution of $3\Gamma_8^-$ and $1\Gamma_7^-$. The ground-state energy of individual acceptors is indicated by a vertical line. Experimental data according to Rotsaert *et al.* (Refs. 8 and 23): D (▽), C (□), B (△), and G (○).

are, however, more extended regarding the number of excited states and the range of ground-state binding energies. In addition we now dispose of absolute experimental data for comparison.

Good agreement is found with most data for the EMA donor in Si and Ge given by Kogan *et al.*[12,13] (the highest states calculated are $4p_{\pm}$ and $4p_0$). A difference appears as the ground state becomes deeper, which obviously is a consequence of the different method to introduce the central-cell correction.

A more substantial difference exists with the acceptor data of Kogan and Polupanov.[14,15] These authors find, e.g., no chemical dependence of the D line f value, in clear disagreement with our experimental findings. Recent calculations of Bingelli and Baldereschi[16] give f values for acceptors in germanium which are close to our calculated data for the gallium acceptor. The latter authors also apply q-dependent dielectric screening and a short-range potential for the ground-state correction as in the present paper; explicit data on the chemical dependence are, however, not given.

TABLE IV. Donors in germanium: experimental f values.

	Donor		
	Sb	P	As
$2p_{\pm}$	0.124	0.063	0.063
$3p_{\pm}$	0.023	0.012	0.014
$4p_{\pm}$	0.007	0.006	0.005
$4f_{\pm}$		0.005	0.004
$2p_0$	0.013	0.007	0.007

TABLE V. Acceptors in germanium: experimental f values.

	Acceptor			
	B	Al	Ga	In
G	0.0025	0.0016	0.0025	0.001
D	0.066	0.053	0.046	0.040
C	0.053	0.036	0.033	0.029
B	0.0047	0.0037	0.0043	0.0047
Ai	0.011	0.010	0.012	0.011
Ii	0.006	0.003	0.006	0.004

When we compare our calculated values with the experimental data, it is obvious that the general structure of the absorption spectrum is very well reproduced. This may, e.g., be demonstrated by the relative intensities of the donor absorption lines. Inspection of Table IV indicates that in germanium the relative intensities of $2p_0$:$2p_{\pm}$:$3p_{\pm}$:$4p_{\pm}$:$4f_{\pm}$ are close to 1:10:2:1:1 and these ratios are also found in the calculated results of Table II and Fig. 2. In silicon the experimental donor spectra show intensities of $2p_0$:$3p_{\pm}$:$4p_{\pm}$:$4f_{\pm}$:$5p_{\pm}$ that are on the

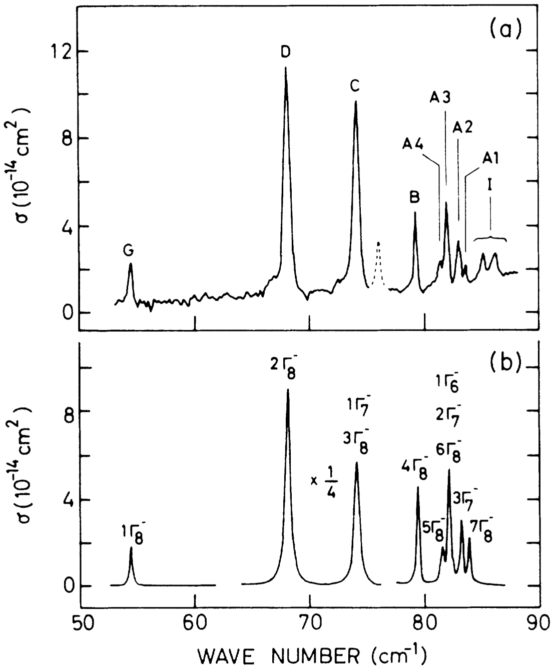

FIG. 4. Experimental (a) and calculated (b) absorption spectrum of the gallium acceptor in germanium. $N_{\mathrm{Ga}} = 8.5 \times 10^{13}$ atoms/cm^3. Experimental resolution is 0.25 cm^{-1}. The dashed peak is due to As (Refs. 8 and 23). The calculated spectrum is a simulation using the gallium data of Table III up to the $7\Gamma_8^-$ transition, each theoretical line position being broadened by a Lorentzian line shape of 0.25 cm^{-1} half-width in order to agree with the experimental resolution (0.50 cm^{-1} was taken for $2\Gamma_8^-$, $3\Gamma_8^-$, and $1\Gamma_7^-$ to account for the observed width of D and C). The contributions of $3\Gamma_8^-$ and $1\Gamma_7^-$ are unresolved giving rise to one single line (C); the same applies to $1\Gamma_6^-$, $2\Gamma_7^-$ and $6\Gamma_8^-$ giving rise to a single $A3$ line. The I lines are not simulated.

average related as 12:10:3:1:2 (see, e.g., Ref. 17, where relative f-values are listed; the $2p_{\pm}$ line is the strongest but a value is not given since the maximum is close to zero transmission). Again a fair correspondence is found with the calculated results of Table I and Fig. 1.

The correspondence for acceptors in germanium is illustrated in Fig. 4, where the experimental gallium spectrum is compared with a simulated spectrum using the calculated gallium data of Table III. Notice that the comparison is absolute since both spectra are reproduced on the same absorption cross section scale. The simulated spectrum has been constructed as a sum of Lorentzian lines with half-widths equal to the experimental resolution (the D and C line have larger widths), and so that the area under the line is proportional to the calculated f value of the transition; the absorption cross section is obtained using formula (2) with N_{imp} the known gallium concentration. Except for the D and C line, which are overestimated by the calculation, the correspondence of the G and B line and of the Ai multiplet is excellent. It is obvious that the Ai multiplet is completely explained by transitions towards odd-parity excited states. The $A3$ line is a composition of three unresolved components with the main contribution from $2\Gamma_7^-$. The C line is also composed of two unresolved lines from $3\Gamma_8^-$ and $1\Gamma_7^-$, with $1\Gamma_7^-$ accounting for most of the intensity; this was also stated by Bingelli and Baldereschi.[16] Inspection of Table III indicates that the assignment to mainly $1\Gamma_7^-$ applies to the whole shallow acceptor range.

The agreement between calculation and experiment regarding the dependence of the f values on the binding energy of the ground state is considered to be fair. The calculations confirm that there is indeed a physical basis for the experimental observation that the absorption cross section of most absorption lines depends on the identity of the shallow impurity.[8] The agreement in the magnitude of the chemical dependence both for donors and acceptors seems to justify the use of the variable screening potential (3), even if such a procedure is not strictly within the limits of the effective-mass approximation.[16] Anyhow the procedure applied here is considered better than the method applied by Kogan *et al.*[12–15] since they failed to predict a substantial chemical dependence for the acceptor D line.

The calculated f values of the strongest transitions exceed the corresponding experimental data, e.g., by 50–100 % for the acceptor D line and by about 60% for the $2p_{\pm}$ donor line to mention the largest deviations. The deviation seems too systematic in order to be entirely accounted for by experimental errors (experimental data from two different sources were used[8,9]). A substantial deviation of the effective-field ratio in (2) from unity is not expected (certainly not for germanium where the wave functions are the most extended) and would render the situation even worse. The most plausible explanation is perhaps that the ground-state wave function is not given to a sufficient accuracy by effective-mass calculations in order to expect perfect agreement.

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