Identification of the Bi_{Ga} heteroantisite defect in GaAs:Bi

M. Kunzer, W. Jost, and U. Kaufmann
Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastrasse 72, W-7800 Freiburg, Federal Republic of Germany

H. M. Hobgood and R. N. Thomas
Westinghouse Science and Technology Center, Pittsburgh, Pennsylvania
(Received 8 December 1992)

GaAs lightly doped with the heaviest group-V atom, bismuth (Bi), has been studied by conventional electron-spin resonance (ESR) and by ESR detected via the magnetic-circular-dichroism (MCD) absorption. A new Bi-related sharp-line MCD band has been observed on which two MCD-ESR lines have been discovered. They are shown to arise from the singly ionized Bi_{Ga} double donor. Most remarkably, a substantial fraction, about 10%, of the total Bi content is found to occupy the Ga site. The Bi_{Ga} MCD absorption band is tentatively assigned to an exciton deeply bound to the singly ionized double donor ${Bi_{Ga}}^+$.

I. INTRODUCTION

In elemental crystalline semiconductors only two basic types of lattice disorder exist: vacancies and interstitials. In binary semiconductors a third type of intrinsic disorder is possible, namely antisite defects. These are misplaced atoms, e.g., an anion on a cation site, or vice versa. These antisite defects were almost completely ignored until the middle of the 1970s.[1] The first reliable experimental evidence for an antisite defect was obtained for the III-V semiconductor GaP, where the P_{Ga} anion antisite defect was identified by electron-spin resonance (ESR).[2] For GaP, GaAs, and InP the anion antisites P_{Ga}, As_{Ga}, and P_{In}, respectively, have become the most reliably identified intrinsic defects.[3,4]

Isovalent (isoelectronic) impurities in GaAs have attracted interest as dopants to reduce the dislocation density of semi-insulating material. In such samples also anion heteroantisites, i.e., non-native group-V dopants on the Ga site, have been discovered, the first example being Sb_{Ga} in GaAs:Sb,[5] and very recently P_{Ga} in GaAs:P.[6] In this paper we report on the identification of the Bi_{Ga} heteroantisite in GaAs:Bi and we show that heteroantisite formation probability in GaAs increases dramatically by five orders of magnitude in the sequence As_{Ga}, Sb_{Ga}, and Bi_{Ga}.

The data to be reported here are mostly based on the magnetic-circular-dichroism (MCD) absorption technique. The MCD absorption is defined as the difference in absorption of right and left circularly polarized light when the sample is placed in an external magnetic field and the light propagates along the field direction. Of particular interest for defect studies is the paramagnetic MCD which is temperature dependent. It arises from the differential optical absorption due to transitions between Zeeman split levels. The paramagnetic MCD signal strength is therefore proportional to the ground-state spin polarization. The technique reveals its full power when combined with microwaves. If the MCD signal is monitored at a fixed photon energy while sweeping the magnetic field, there will be a change in the MCD signal at resonance since the microwave transitions change the ground-state spin polarization. This change is the MCD-ESR signal. In many cases MCD-ESR is considerably more sensitive than conventional ESR.

II. EXPERIMENTAL DETAILS

The GaAs:Bi crystals used for this study were grown by the liquid encapsulation Czochralski technique from a bismuth-doped melt. A secondary-ion mass spectroscopy analysis of the pulled crystal indicates a Bi concentration of 2.6×10^{16} cm^{-3} corresponding to an effective segregation coefficient of around 1×10^{-4} for Bi in GaAs. Hall-effect analysis of this material shows semi-insulating behavior with resistivities in the mid 10^7 Ω cm range and a mobility of about 5800 cm^2/V s at 300 K.

Conventional ESR measurements were performed at 9.55 GHz using 100-KHz field modulation and lock-in detection. The samples were mounted in a liquid-He continuous-flow cryostat. A K-band (18–26 GHz) optically detected magnetic-resonance setup built around a 4-T superconducting split-coil magnet was used for magnetic-circular-dichroism absorption and MCD-ESR studies.

III. RESULTS

It was first attempted to observe ESR lines attributable to Bi_{Ga} by conventional ESR at 9.55 GHz. No such signal was found up to fields of 1.75 T in this early stage but the GaAs:Bi samples revealed the four-line ${As_{Ga}}^+$ hyperfine pattern between 0.15 and 0.44 T already in the dark.

In the next step, the MCD absorption of a GaAs:Bi sample was measured. A spectrum is shown in Fig. 1 and it is readily recognized to be a superposition of the well-known As_{Ga} $EL2^+$ MCD absorption band[7] and a new, sharply structured band between 1.1 and 1.2 eV. Figure

0163-1829/93/48(7)/4437(5)/$06.00 ©1993 The American Physical Society

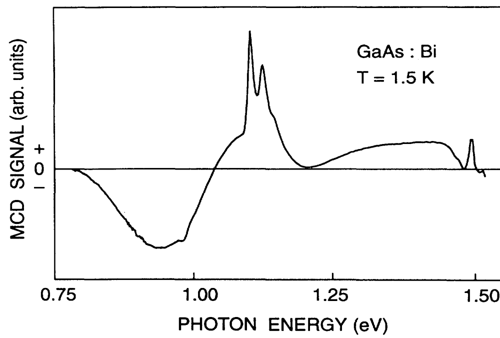

FIG. 1. Overall MCD absorption band of GaAs:Bi containing contributions from As_{Ga} $EL2^+$ and $Bi_{Ga}{}^+$.

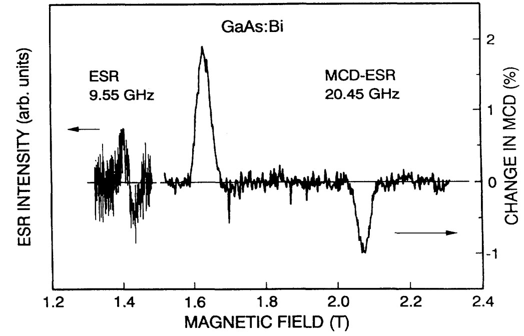

FIG. 3. MCD-ESR (1.5 K) and conventional ESR (4.2 K) spectra of GaAs:Bi. The 9.55-GHz ESR trace is an average of 10 individual scans.

2 shows this band with better spectral resolution (1 meV) following persistent quenching of the As_{Ga} $EL2^+$ MCD band with $h\nu = 1.18$ eV light (metastabilization of As_{Ga} $EL2$). The band consists of a 10-meV broad zero-phonon line (ZPL) at 1.103 eV and replicas at 21, 25, 44, 61, 77, and 93 meV from the ZPL.

MCD-ESR spectra were taken at 20.45 GHz by measuring microwave-induced changes of the MCD absorption at a fixed photon energy as a function of magnetic field. For photon energies in the range 0.8 eV $< h\nu <$ 1.4 eV, the four-line MCD-ESR spectrum of $As_{Ga}{}^+$ is observed in the field range 0.55–0.83 T. In addition, two new, isotropic MCD-ESR lines are observed on the structured band of Fig. 2. They occur at 1.63 and 2.06 T, see Fig. 3, and have a width of 43 mT. If the microwave frequency is slightly increased the 1.63-T line moves to lower fields while the 2.06-T line moves to higher fields. The microwave-induced changes of the MCD recover, at 1.5 K, to the equilibrium MCD value with a time constant of about 4 s when the microwaves are switched off. This very long spin-lattice relaxation time indicates that the ground state of the defect in question is s-like in character. It is now demonstrated that the two MCD-ESR lines can be consistently assigned to the Bi_{Ga} double donor in its singly ionized charge state $Bi_{Ga}{}^+$.

IV. DISCUSSION

In analogy with As_{Ga} and Sb_{Ga} in GaAs,[4,5,8] Bi_{Ga} is expected to be a double donor. Therefore the singly ionized donor, $Bi_{Ga}{}^+$, should have a paramagnetic ground state with an s-like orbital part of the wave function. As a consequence, one expects a strong isotropic Fermi contact hyperfine (hf) interaction between the electron spin $S=\frac{1}{2}$ and the bismuth nuclear spin $I=\frac{9}{2}$ for ^{209}Bi, the only stable bismuth isotope. Thus, the spin Hamiltonian describing the ground-state interactions in an external magnetic field H contains the Zeeman and the hf interactions and has the form

$$\mathcal{H} = g\mu_B \mathbf{H}\cdot\mathbf{S} + A\,\mathbf{I}\cdot\mathbf{S}\ .$$

In the above Hamiltonian, μ_B is the Bohr magneton. The g factor and the hf constant A are parameters to be determined from the ESR spectrum. In zero magnetic field the hf interaction splits the $Bi_{Ga}{}^+$ ground state into two states of total angular momenta $F = I \pm S = 4$ or 5, respectively, separated by $5A$. In a magnetic field these states are split and their energies are given by the eigenvalues of the above Hamiltonian for which simple analytical solu-

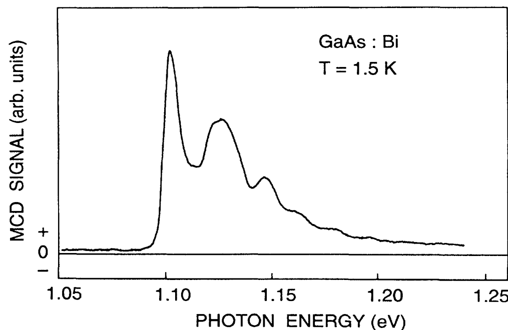

FIG. 2. The $Bi_{Ga}{}^+$ MCD absorption band following quenching of the As_{Ga} $EL2^+$ MCD band.

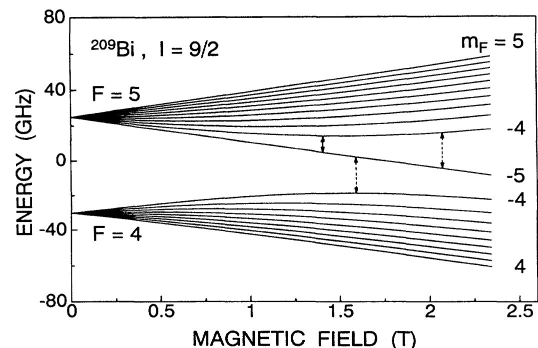

FIG. 4. Breit-Rabi diagram for the $Bi_{Ga}{}^+$ ground state. Microwave transitions observed at 20.45 and 9.55 GHz are shown as dashed and full arrows, respectively.

TABLE I. Parameters for group-V antisites in GaAs.

	g	A (GHz)	A/A_f	Formation probability f	(0/+) level below E_c (eV)
P_{Ga}	1.99	1.80	0.140		
As_{Ga}	2.04	2.70	0.184	$\sim 10^{-6}$	0.75
$^{121}Sb_{Ga}$	2.02	6.61	0.188	$\sim 10^{-3}$	0.48
Bi_{Ga}	2.055	10.96	0.141	$\sim 10^{-1}$	0.35–0.50

tions exist.[9] They are plotted in the Breit-Rabi diagram of Fig. 4. With g and A as listed in Table I for Bi_{Ga}, the two allowed ($\Delta m_F = \pm 1$) microwave transitions at 20.45 GHz, shown as the dashed line in Fig. 4, provide a fit to the two MCD-ESR lines in Fig. 3, and are accurate to within 5 mT. We therefore assign these lines to the Bi_{Ga} antisite. The experimental error in g and A is 0.005 and 0.05 GHz, respectively.

It is noted that the above assignment is consistent with the observed change in resonance fields of the two MCD-ESR lines when the microwave frequency is slightly increased. Second, a g value close to the free-electron value (2.002) is what one expects for an s-like ground state. Finally, it is now demonstrated by a scaling procedure that the hf-parameter A deduced from the spectrum is reasonable also. Listed in Table II are the hf parameters of the group-V antisites in GaAs, $V_{Ga}{}^{+}$, the doubly negative group-V hexafluoride radicals, $VF_6{}^{2-}$,[10] and of the fourfold ionized group-V free atoms, V^{4+}.[11] As for the free V^{4+} ions, the electron configuration of the group-V element in the hexafluorides is ns^1. In an ionic picture, the charge state of a singly ionized group-V antisite double donor in GaAs is also V^{4+} with an ns^1 configuration. One can therefore use the ratio $A(As_{Ga}{}^{+})/A(AsF_6{}^{2-}) = 0.287$ for scaling the A values of $SbF_6{}^{2-}$ and $BiF_6{}^{2-}$ to obtain estimates of A for $Sb_{Ga}{}^{+}$ and $Bi_{Ga}{}^{+}$. These values are given in brackets in Table II and to within 10% agree with the hf parameters determined experimentally. Thus, the $Bi_{Ga}{}^{+}$ assignment is sound.

The microwave transition observed by MCD-ESR within the $F=5$ manifold should also be observable by conventional ESR at 9.55 GHz, see the short arrow in Fig. 4. Once g and A are known from the K-band MCD-ESR data, the resonance field at 9.55 GHz can be predicted accurately. It should occur at 1.42 T. The ESR spectrum, therefore, has been remeasured between 1.3 and 1.5 T using signal-averaging techniques. The 9.55-GHz trace in Fig. 3 is an average of 10 individual scans. A weak isotropic line at 1.42 T with a peak-to-peak width of 35 mT (true width 42 mT) is, in fact, observed already in the dark. This finding provides the final confirmation for the $Bi_{Ga}{}^{+}$ model.

Most often, MCD-ESR lines correspond to a decrease in MCD absorption intensity as for the 2.06-T line in Fig. 3, since microwave transitions usually destroy the spin polarization partially and thus the paramagnetic MCD. A sign reversal, as for the 1.63-T line in Fig. 3, has been reported occasionally, e.g., in the MCD-ESR spectra of Fe^{3+} in InP (Refs. 12 and 13) and for the $Bi_{Me}{}^{4+}$ defect in $Bi_{12}MO_{20}$ (M=Si, Ge, Ti) sillenite crystals.[14] For InP:Fe^{3+} optical pumping effects have been invoked[12] to explain the effect. Although optical pumping can lead to a ground-state population inversion,[15] this explanation is inadequate in the present case. Alternatively, for InP:Fe^{3+} the effect has been ascribed[13] to specific spin-lattice relaxation mechanisms. A similar model has been proposed for Bi_M in sillenites.[14] Here we suggest still another but very simple and transparent explanation. The MCD absorption intensity at a fixed photon energy as a function of the magnetic field is a measure for the total ground-state electron-spin polarization P which is the sum of the individual contributions from all occupied Zeeman levels, in the present case all (F,m_F) levels in Fig. 4. For such an individual contribution $P_{F,m}$, the following proportionality holds:[16]

$$P_{F,m} \propto -\frac{\partial E_{F,m}}{\partial H} \exp\left[-\frac{E_{F,m}}{kT}\right],$$

where $E_{F,m}$ is the energy of the level (F,m_F), all other symbols having their usual meaning. The above relation reveals that Zeeman levels with a positive (negative) slope versus H give a negative (positive) contribution to the total polarization. In particular, for a vanishing slope there is no contribution to the polarization. Therefore, a microwave transition starting from a level with zero slope and ending in a level with negative slope necessarily *increases* the total polarization and thus the MCD intensity. The only condition is that the occupation of the lower level is higher than that of the upper one. Of course, this is the case in thermal equilibrium. This situation is seen to occur for the 1.63-T transition in Fig. 4. It is suggested that this is the basic mechanism producing enhancing MCD-ESR signals. Analogous considerations immediately show that the 2.06-T transition quenches the MCD intensity.

The $Bi_{Ga}{}^{+}$ concentration estimated from the ESR in-

TABLE II. Hyperfine parameters A in GHz for $V_{Ga}{}^{+}$ antisites in GaAs and tetravalent group-V ions.

	^{75}As	^{121}Sb	^{209}Bi
$V_{Ga}{}^{+}$	2.70[a]	6.61[a] (6.14)[b]	10.96[c] (10.35)[b]
$(VF_6{}^{2-})$[d]	9.40	21.39	36.02
A_f[e]	14.66	35.10	77.53

[a]Reference 5.
[b]Predicted by scaling, see text.
[c]This work.
[d]Reference 10.
[e]Calculated value for a free-ion ns electron, Ref. 11.

tensity is around 3×10^{15} cm^{-3}. This small concentration explains why the $Bi_{Ga}{}^{+}$ ESR line was not observed in the initial attempt. On the other hand, this $Bi_{Ga}{}^{+}$ concentration is large in view of the total Bi concentration of the sample, 2.6×10^{16} cm^{-3}. If an antisite formation probability f is defined as the ratio of group-V antisite concentration and the total group-V atom concentration, one finds a dramatic increase of f with increasing group-V atomic number. For the intrinsic As_{Ga} defect in GaAs f is around 10^{-6},[4] for Sb_{Ga} it is around 10^{-3},[5] and for Bi_{Ga} it is near 10^{-1}, see Table I. Most likely, this increase is a consequence of the decreasing electronegativity in the sequence As, Sb, Bi. Size effects, on the other hand, seem to play a minor role.

It has not been possible to measure the positions of the two Bi_{Ga} donor levels, e.g., by photo-ESR. However, rough estimates can be obtained in the following way. According to the electrical specifications of the sample and to the fact that ESR of $As_{Ga}{}^{+}$ is observed in the dark, it is clear that the Fermi level is pinned to the midgap position, i.e., 0.75 eV below the conduction-band edge E_c. From the known trend for the chalcogen double donors S, Se, Te in silicon[17] and from theoretical predictions,[18–20] one expects for the group-V double donors on a Ga site in GaAs that both donor levels become shallower in the sequence As_{Ga}, Sb_{Ga}, and Bi_{Ga}. For Sb the second level $(+/++)$ is at $E_c-0.7$ eV.[8] The corresponding Bi_{Ga} level cannot be significantly shallower since this would prevent observation of the $Bi_{Ga}{}^{+}$ ESR and MCD-ESR in the dark. Therefore the $Bi_{Ga}(+/++)$ level should be in the range 0.7–0.65 eV below E_c.[21] The first donor level of a double donor in tetrahedrally bonded semiconductors is typically 0.2–0.3 eV above the second level.[17,22] Thus, the $Bi_{Ga}(0/+)$ level is expected in the range 0.35–0.50 eV below E_c.

Apart from the parameters discussed above, Table I also contains a column for A/A_f which is a measure for the density of the second donor electron at the central atom of the antisite in question.[5] This density for $Bi_{Ga}{}^{+}$ is smaller than for $As_{Ga}{}^{+}$ or $Sb_{Ga}{}^{+}$ but still typical for group-V antisites in III-V compounds. In this connection it is also instructive to note that the bismuth Fermi contact interaction decreases from the free-ion value $A_f=77.5$ GHz to 36.0, 19.2, and 10.9 GHz in sixfold fluorine coordination,[10] sixfold oxygen coordination,[14] and fourfold As coordination, respectively. Of course, this trend reflects the decreasing ionicity of the ligands.

The $Bi_{Ga}{}^{+}$ MCD-ESR is observed only on the MCD absorption band in Fig. 2. Therefore the band must be related to Bi_{Ga} and the initial state of the optical transition responsible for it must be the $Bi_{Ga}{}^{+}$ ground state. The shape of the $Bi_{Ga}{}^{+}$ band is, however, very different from the As_{Ga} $EL2^{+}$ (Ref. 7) and the $Sb_{Ga}{}^{+}$ (Refs. 23 and 24) MCD bands. They have a spectral extent exceeding that of the $Bi_{Ga}{}^{+}$ band by about a factor of 7 and they do not reveal any sharp structures. This broadband character is one strong argument for the involvement of ionizing transitions in the MCD absorption of As_{Ga} $EL2^{+}$ and $Sb_{Ga}{}^{+}$.[23,25] Nevertheless, other authors[26] for As_{Ga} $EL2^{+}$ prefer an interpretation in terms of an internal $A_1\rightarrow T_2$ transition. The characteristics of the $Bi_{Ga}{}^{+}$ MCD band reveal that an ionizing transition, in this case, is very unlikely. It is therefore proposed that the $Bi_{Ga}{}^{+}$ MCD absorption is due to the creation of an exciton at $Bi_{Ga}{}^{+}$ according to the reaction $Bi^{+}+h\nu\rightarrow Bi_{Ga}{}^{+}X$. This interpretation is suggested by the striking similarity of the $Bi_{Ga}{}^{+}$ MCD band and those of excitons bound to neutral shallow donors in GaP.[27] The $Bi_{Ga}{}^{+}X$ bound exciton can be viewed as $Bi_{Ga}{}^{0}h$ with the electron deeply bound in the $Bi_{Ga}(0/+)$ donor level and with the hole h weakly bound to the neutral Bi_{Ga} donor. In this model hole binding must result from a short-range potential, possibly mediated by the strain field induced by the expected very large, totally symmetric outward relaxation of the As ligands surrounding Bi_{Ga}. The exciton model is consistent with the energetic position of the 1.103-eV zero-phonon line in the $Bi_{Ga}{}^{+}$ MCD spectrum. Neglecting the hole binding energy and using the above estimate for the $Bi_{Ga}(0/+)$ level position one finds that the $Bi_{Ga}{}^{+}$ exciton ZPL should occur between 1.17 and 1.02 eV. Although the excitonic model for the $Bi_{Ga}{}^{+}$ MCD band is appealing it needs further confirmation, in particular since the $A_1\rightarrow T_2$ internal transition model for Bi_{Ga} also has appealing features. One difficulty with the latter model, connected with the enormous spin-orbit coupling of bismuth p electrons (e.g., $\Delta_{so}=2.58$ eV for the Bi^{2+}, configuration s^2p^1, free-ion ground state), is, however, evident. The calculated $A_1\rightarrow T_2$ splitting is very close to 1.0 eV for the P_{Ga}, the As_{Ga}, and the Sb_{Ga} antisites in GaAs.[19,20] Assuming the same splitting for Bi_{Ga}, the spin-orbit interaction within the $^2T_2$ state may reduce the separation between the spin-orbit levels Γ_6 $(^2A_1)$ and Γ_7 $(^2T_2)$ to a value much too small to account for the position of the 1.103-eV zero-phonon line.

V. CONCLUSION

Semi-insulating GaAs doped with Bi to a level of 2.6×10^{16} cm^{-3} has been studied by conventional ESR, MCD, and MCD-ESR. The MCD-ESR together with the ESR results unambiguously demonstrate the existence of Bi_{Ga} antisite defects. Their concentration amounts to about 10% of the total Bi concentration, and it is concluded that antisite formation probability in GaAs increases by five orders of magnitude in the sequence As_{Ga}, Sb_{Ga}, Bi_{Ga}. Estimates for the two levels of the Bi_{Ga} double donor are given. A simple explanation for the occurrence of enhancing MCD-ESR signals is presented.

The shape of the observed Bi_{Ga} MCD absorption band is qualitatively different from those reported for all other anion antisites in III-V compounds. It is suggested that the optical transition giving rise to the MCD band, in the present case, involves an exciton deeply bound to $Bi_{Ga}{}^{+}$.

ACKNOWLEDGMENTS

We are grateful to K. Sambeth for expert technical assistance. We thank W. Jantz and J. Schneider for useful discussions and H. J. Reyher for sending us a copy of Ref. 14 prior to its publication.

[1] J. A. Van Vechten, J. Electrochem. Soc. **122**, 423 (1975).
[2] U. Kaufmann, J. Schneider, and A. Räuber, Appl. Phys. Lett. **29**, 312 (1976).
[3] A. N. Georgobiani and I. M. Tiginyanu, Fiz. Tekh. Poluprovodn. **22**, 3 (1988) [Sov. Phys. Semicond. **22**, 1 (1988)].
[4] U. Kaufmann, in *Festkörperprobleme, Advances in Solid State Physics,* edited by U. Rössler (Vieweg, Braunschweig, 1989), Vol. 29, p. 183; for P_{In} in InP see T. A. Kennedy, E. R. Glaser, B. Molnar, and M. G. Spencer, in *Defect Control in Semiconductors,* edited by K. Sumino (North-Holland, Amsterdam, 1990), p. 975.
[5] M. Baeumler, J. Schneider, U. Kaufmann, W. C. Mitchel, and P. W. Yu, Phys. Rev. B **39**, 6253 (1989).
[6] M. Jordan, T. Hangleiter, and J. M. Spaeth, Semicond. Sci. Technol. **7**, 738 (1992).
[7] B. K. Meyer, H. M. Spaeth, and M. Scheffler, Phys. Rev. Lett. **52**, 851 (1984).
[8] P. Omling, B. H. Yang, L. Samuelson, R. Yakimova, J. O. Fornell, and L. Ledebo, Phys. Rev. B **44**, 13 398 (1991).
[9] G. Breit and I. I. Rabi, Phys. Rev. **38**, 2082 (1931).
[10] A. R. Boate, J. R. Morton, and K. F. Preston, J. Phys. Chem. **82**, 718 (1978).
[11] J. R. Morton and K. F. Preston, J. Magn. Magn. Res. **30**, 577 (1978).
[12] I. R. Agool, M. Deiri, and B. C. Cavenett, Semicond. Sci. Technol. **4**, 48 (1989).
[13] A. Görger and J. M. Spaeth, Semicond. Sci. Technol. **6**, 800 (1991).
[14] H. J. Reyher, U. Hellwig, and O. Theimann, Phys. Rev. B **47**, 5638 (1993).
[15] R. Bernheim, *Optical Pumping—An Introduction* (Benjamin, New York, 1965).
[16] J. H. Van Vleck, *The Theory of Electric and Magnetic Susceptibilities* (Oxford University, New York, 1965).
[17] E. Janzén, R. Stedman, G. Grossmann, and H. G. Grimmeiss, Phys. Rev. B **29**, 1907 (1984).
[18] H. P. Hjalmarson, P. Vogl, D. J. Wolford, and J. D. Dow, Phys. Rev. Lett. **44**, 810 (1980).
[19] M. J. Caldas, J. Dabrowski, A. Fazzio, and M. Scheffler, Phys. Rev. Lett. **65**, 2046 (1990).
[20] M. J. Caldas, J. Dabrowski, A. Fazzio, and M. Scheffler, in *Proceedings of the 20th International Conference on The Physics of Semiconductors,* edited by E. M. Anastassakis and J. D. Joannopoulos (World Scientific, Singapore, 1990), p. 469.
[21] In a perfectly homogeneous semi-insulating GaAs crystal, ESR of $Bi_{Ga}{}^{+}$ would not be observable in the dark if the $Bi_{Ga}(+/++)$ level is above E_F. It is, however, well known that state-of-the-art semi-insulating GaAs material is spatially inhomogeneous. This leads to spatial fluctuations of the band edges and impurity levels relative to E_F. From local resistivity variations quoted for semi-insulating GaAs in the literature one estimates that the amplitude of the potential fluctuations is less than 100 meV. This estimate leads to the $E_c - 0.65$ eV limit for the $Bi_{Ga}(+/++)$ level.
[22] G. B. Bachelet, M. Schlüter, and G. A. Baraff, Phys. Rev. B **27**, 2545 (1983).
[23] P. Omling, D. M. Hoffmann, M. Kunzer, M. Baeumler, and U. Kaufmann, Phys. Rev. B **45**, 3349 (1992).
[24] B. Bohl, M. Kunzer, F. Fuchs, G. Hendorfer, and U. Kaufmann, Phys. Rev. B **46**, 10 450 (1992).
[25] U. Kaufmann and J. Windscheif, Phys. Rev. B **38**, 10 060 (1988).
[26] K. Krambrock, J. M. Spaeth, C. Delerue, G. Allan, and M. Lannoo, Phys. Rev. B **45**, 1481 (1992).
[27] J. J. Lappe, B. K. Meyer, and J. M. Spaeth, in *Proceedings of the International Conference on Shallow Impurities in Semiconductors,* edited by B. Monemar, IOP Conf. Proc. No. 95 (Institute of Physics and Physical Society, London, 1989), p. 249.