Optical characterization of a deep (Cu-C)-related complex defect in GaP

W. M. Chen, B. Monemar, and M. Godlewski*
Department of Physics and Measurement Technology, Linköping University, S-581 83 Linköping, Sweden
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A complex neutral defect with an associated deep bound exciton (BE) at ~ 1.4 eV in GaP has been studied with photoluminescence and optically detected magnetic resonance (ODMR). This defect has been observed after diffusing Cu at ~ 850–$1050\,^{\circ}$C into C-rich GaP and is believed to contain both C and Cu. The lowest electronic excited state of this deep BE is a magnetic triplet, which can be described with a spin-triplet spin Hamiltonian $H_S=\mu_B \mathbf{B}\cdot\underline{\mathbf{g}}\cdot\mathbf{S}+\mathbf{S}\cdot\underline{\mathbf{D}}\cdot\mathbf{S}+\mathbf{S}\cdot\underline{\mathbf{A}}\cdot\mathbf{I}+\sum_i \mathbf{S}\cdot\underline{\mathbf{A}}_i\cdot\mathbf{I}_i$. The fit of this Hamiltonian to the experimental ODMR data gives the parameter values $g_x=g_y=1.97\pm0.05$, $g_z=2.00\pm0.05$, $D_x=D_y=(-0.78\pm0.10)\times10^{-5}$ eV, $D_z=(1.56\pm0.10)\times10^{-5}$ eV, where the principal (axial) defect axis $\underline{\mathbf{z}}$ diagonalizing both the $\underline{\mathbf{g}}$ tensor and the $\underline{\mathbf{D}}$ tensor simultaneously is along $\langle 111\rangle$. In the fitting procedure it was necessary to include hyperfine interactions of size $\sim 1.3\times10^{-6}$ eV in order to obtain a satisfactory fit, although they are not resolved in the broad ODMR spectra. The defect symmetry is deduced to be C_{3v} and its identity is suggested to be a $\langle 111\rangle$-oriented three-atom complex, with a C_{Ga} and a Cu_{Ga} as the dominating donorlike and acceptorlike potentials, respectively, in addition to an adjacent shallow donor (probably Cu_i). The isolated C_{Ga} donor has not been observed in this work, but the above model for the 1.4-eV defect leads to a binding energy for C_{Ga} of at least 0.7 eV, consistent with theoretical calculations.

I. INTRODUCTION

C substituted on the P site in GaP is known to be a shallow "hydrogenic" acceptor,[1–3] with a binding energy of about 54 meV.[3] The substitutional C on the Ga site in GaP is naturally supposed to be a donor, but apparently has so far not been identified. Theoretical Green's-function calculations have predicted that C_{Ga} should give a deep A_1-like donor level in the band gap.[4]

When C-rich GaP is Cu-diffused, at least two different complex defects related to both Cu and C are formed, under varying conditions of diffusion. One such defect produced by diffusing Cu at 850–900 °C in GaP gives a bound-exciton (BE) spectrum at 2.238 eV at 2 K (Ref. 5) and is assumed to involve interstitial C in addition to Cu_{Ga}.[5] With slightly higher diffusion temperatures, another deeper BE spectrum appears, peaking at about 1.4 eV, which replaces the one observed with lower Cu diffusion temperatures. This photoluminescence (PL) band is broad and featureless due to strong phonon coupling, and no electronic lines can be observed, unfortunately.

In contrast to the 2.238-eV (Cu-C)-related BE, which does not show any optically detected magnetic resonance (ODMR) in spite of a triplet configuration as the lowest BE state, the 1.4-eV system shows quite strong ODMR signals. This gives information on the microscopic structure of the defect. Such information is in this case not accessible by other more conventional techniques of perturbation spectroscopy, such as Zeeman and uniaxial-stress measurements, due to the broad and featureless optical spectrum for the defect. It is argued from a combination of information from the doping procedure and the ODMR results [e.g., the angular dependence and the hyperfine- (hf) related line shape of the ODMR] that this $\langle 111\rangle$-oriented axial defect consists of a C_{Ga}, and in addition a Cu_{Ga} and a Cu_i along a $\langle 111\rangle$ axis.

This paper is organized in the following way. In Sec. II a brief description of the procedure for sample preparation is given, as well as for the experimental measurements. Section III contains a description of optical and ODMR spectra, the latter evaluated with a spin-triplet spin Hamiltonian. In Sec. IV the electronic structure and identity of the defect are discussed in more detail, in relation to the defect-formation process. Comparison is also made with other similar neutral deep-level defects in GaP. In Sec. V some very brief conclusions are summarized.

II. SAMPLES AND EXPERIMENTAL PROCEDURE

As the starting material for preparing the samples, solution-grown GaP crystals were used, which were C doped during the growth. All samples used in this study were originally grown in closed quartz ampoules, either in vacuum or at a CO pressure of up to 150 Torr. In the former case, C is easily introduced accidentally, or is present from the polycrystalline source material, in concentrations in the 10^{16}-cm^{-3} range[1] when C-related luminescence is readily detected close to the band gap [see Fig. 1(a)]. In cases of CO doping, considerably higher C-doping levels are achieved, typically in the 10^{17}-cm^{-3} range for a CO partial pressure of 50–150 Torr in the ampoule.[1] Other residual dopants in the material are N and S, in concentrations estimated to be below 10^{16} cm^{-3}, from the appearance of PL spectra. Due to the irregular shape of the crystals, electrical measurements were not performed in this work.

For Cu doping a diffusion source of Cu was first evaporated on the samples. These were subsequently placed

in quartz ampoules, evacuated and sealed, and diffused at various temperatures in the range 700–1050 °C for about 1 h, followed by a rapid quenching in water to room temperature. This diffusion is estimated from previous experience to introduce a total Cu concentration varying between 10^{16} and 10^{17} cm^{-3}.[5] By this procedure a range of samples with different relative concentrations of Cu and C were obtained. The two (Cu-C)-related defects referred to in this work were only observed in C-rich samples, after Cu diffusion at temperatures above 700 °C. None of these defects were observed in samples doped with C only, or in samples which were only Cu doped but contained a low C concentration.

Cu diffusions at temperatures T_D above 700 °C but lower than 850 °C did not produce the (Cu-C) center discussed in this work. In the range $850 < T_D < 900$ °C the shallow (Cu-C)-related 2.238-eV defect still dominates, but the concentration of the deep 1.4-eV Cu-C center studied in this work increases with an increase in T_D. Rather high Cu-diffusion temperatures in the range 950–1050 °C were necessary to produce samples suitable to study the deep (Cu-C) defect; actually the highest PL intensities of the 1.4-eV PL band were observed for $T_D = 1050$ °C.

In the photoluminescence measurements the samples were immersed in pumped liquid He to reach temperatures below 2 K, and were excited with the 5145-Å line of an Ar^+ laser. The spectra were dispersed through a Spex Industries 1404 double monochromator and detected with an S-20 photomultiplier or a cooled North Coast EO-817 Ge detector. ODMR measurements were performed with a modified Bruker 200-SRC ESR spectrometer, equipped with a cylindrical cavity with optical access from all directions. The sample temperature could be controlled between 2 K and room temperature with a continuous-flow Oxford Instruments liquid-He Crysostat. The ODMR spectra were detected with a North Coast EO-817 Ge detector. A Jobin-Yvon 0.25-m grating monochromator was used to obtain the spectral dependence of the ODMR signals.

III. EXPERIMENTAL RESULTS

In Fig. 1 a typical PL spectrum of a (Cu-C)-doped GaP crystal is shown. In the near-band-gap region, well-known BE spectra related to C_P and other shallow unintentional dopants are observed.[6] Cu-related features are also present, dominated by the 2.177-eV characteristic-orange-luminescence (COL) spectrum.[7] In the infrared (ir) region two emission bands are observed. The first one is a structured band peaking at ~ 1.35 eV, and the second has the peak at 0.85 eV. The band associated with Cu-C in this spectrum peaks at about 1.4 eV (~ 1.38 eV), and overlaps with the O-related donor-acceptor–pair emission peaking at 1.35 eV.[8,9] This 1.4-eV PL band was only found in Cu-diffused GaP with a high C content, which strongly suggests that it is connected with a (Cu-C)-related complex defect. The 0.85-eV band is not consistently observed for GaP crystals doped with C only, and its origin is presently unknown.

The ODMR experiments were performed with detection in the entire spectral region of Fig. 1, but strong resonance signals were only observed for the 1.4-eV band, which as argued here is Cu-C related. This is demonstrated in Fig. 2, which shows the spectral dependence (ODMR-PL) of the ODMR signals (see Fig. 3), compared to an ordinary PL spectrum taken with the same spectral resolution in the same limited spectral region. The broad band detected in the ODMR-PL experiments has a no-phonon region at about 1.45 eV at 4 K [Fig. 2(a)] and a half-width of about 0.1 eV, due to phonon coupling. A comparison between Figs. 2(a) and 2(b) shows that in the PL spectrum there is an overlapping emission due to the O-related *D-A*–pair emission peaking at about 1.35 eV,[8,9] which is not participating in the ODMR.

In Fig. 3 is shown an ir ODMR spectrum of a (Cu-C)-doped GaP crystal at 4 K, for the magnetic field $\mathbf{B}\|[111]$ and in the range $0 < B < 0.6$ T. The resonances are quite

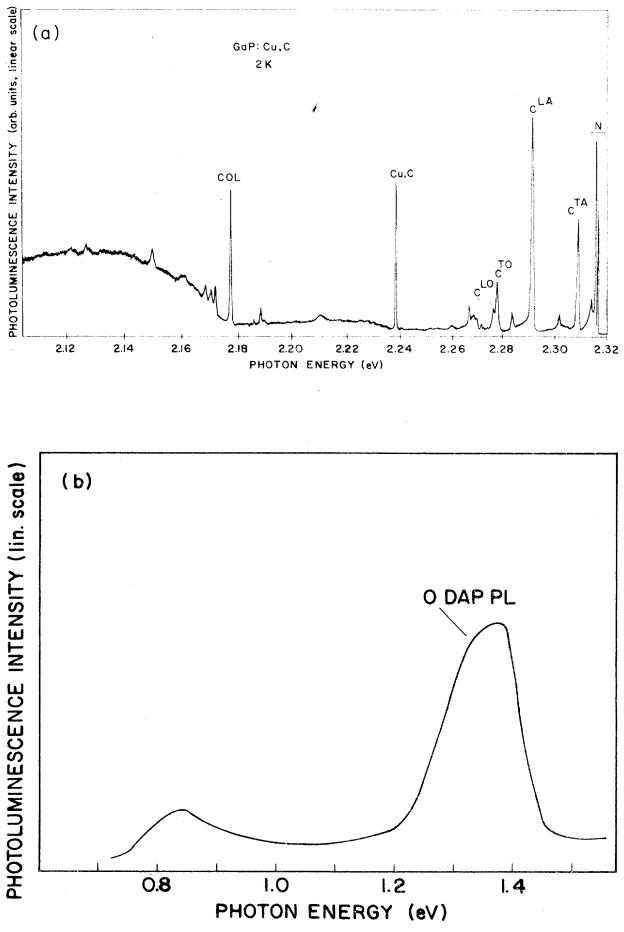

FIG. 1. (a) A high-resolution photoluminescence spectrum of GaP:C, Cu in the visible range. This spectrum is measured for a GaP:C crystal which was copper diffused at 850 °C for 1 h. For higher diffusion temperatures the 2.238-eV C-related BE spectra in (a) gradually disappear. (b) The PL spectrum in the range of the Ge detector for the same sample.

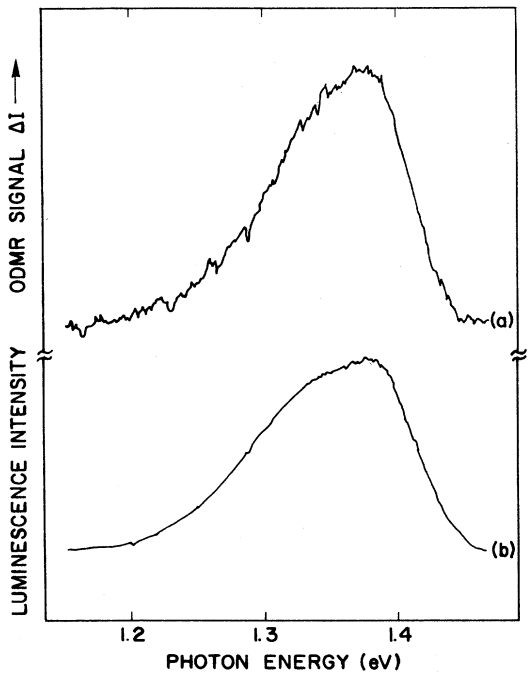

FIG. 2. (a) The spectral dependence of the ODMR signal (ODMR-PL). (b) The PL spectrum measured in the same spectral region and with the same spectral resolution as the ODMR-PL spectrum, for comparison. Spectrum (b) was measured in the same experimental setup used for the ODMR-PL investigations.

strong but broad, as often found in ODMR data for triplet BE's in GaP. The typical resonance linewidth is about 600 G (Fig. 3). The spectrum was taken in the Voigt configuration, and it was observed that the σ and π polarizations in this configuration gave quite similar spectra, due to strong polarization mixing believed to arise from a strong coupling between the substates of the bound exciton, as will be discussed below. The appearance of the ODMR spectrum is well explained in terms of resonances in an $S=1$ triplet system, where the "$\Delta M_S=1$" and "$\Delta M_S=2$" resonances occur with comparable intensities, as also observed for other low-symmetry Cu-related complex defects in GaP.[10-13]

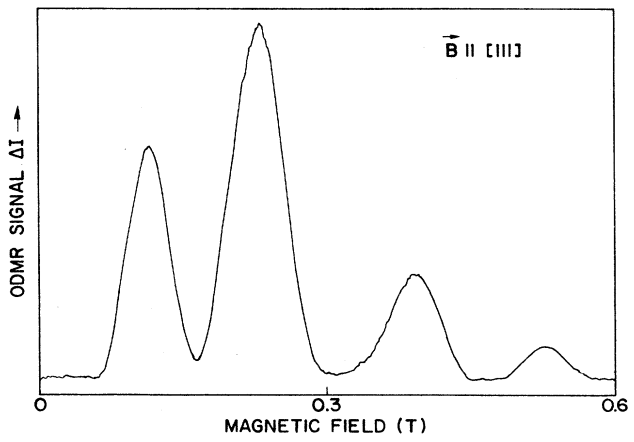

FIG. 3. ODMR spectrum obtained for the 1.4-eV BE system, measured at 4 K and 9.22 GHz with the magnetic field **B** along the [111] axis. This spectrum was measured as a change of the total PL intensity in the resonance, in the Voigt configuration.

The angular dependence of the ODMR spectrum shown in Fig. 3 was measured with **B** rotated in a {110} plane. The angular dependence spectrum is shown in Fig. 4. The data points in Fig. 4 show the peak positions of the stronger resonance lines, where dots are not shown when the lines overlap to an extent that the exact peak positions could not be determined. The $\Delta M_S=1$ lines show a strong anisotropy while the positions of the $\Delta M_S=2$ lines vary very little with angle, as expected in the case of an $S=1$ BE system and in accord with our previous experience.[11-13] This angular dependence was analyzed in terms of a spin-triplet spin Hamiltonian[14]

$$H_S=\mu_B \mathbf{B}\cdot\underline{\mathbf{g}}\cdot\mathbf{S}+\mathbf{S}\cdot\underline{\mathbf{D}}\cdot\mathbf{S}+\mathbf{S}\cdot\underline{\mathbf{A}}\cdot\mathbf{I}+\sum_i \mathbf{S}\cdot\underline{\mathbf{A}}_i\cdot\mathbf{I}_i\ , \qquad (1)$$

where **S** denotes the electronic spin of the BE ($S=1$ for a BE spin triplet). μ_B is the Bohr magneton and **B** the external magnetic field. The first term is the electronic Zeeman term for an electron-hole pair (BE) in its spin-triplet state, and the second term describes the triplet zero-field splitting, originating from magnetic dipole-dipole interaction between the electron and hole, and/or spin-orbit-induced interactions for the bound particles (anisotropic exchange interaction and "classical" fine-structure interaction[14]). The last two terms are the central and ligand hyperfine- (hf) interaction terms, where **I** and $\mathbf{I}_i$ are the nuclear spins of the defect and its ligand atom(s), respectively.

A numerical fit of the spin Hamiltonian to the experimental data is represented by the solid lines in Fig. 4. In the fitting of the above Hamiltonian to the experimental

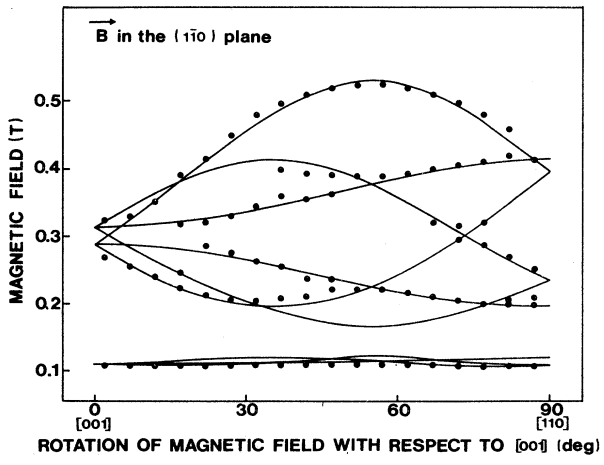

FIG. 4. The angular dependence of the 1.4-eV BE ODMR spectrum, measured with the sample rotated in the (110) plane. The dots show experimental results, while the solid lines are the center of gravity of the broadened hyperfine-unresolved ODMR positions, calculated with the aid of the spin Hamiltonian, with the parameters given in Table I.

TABLE I. Spin Hamiltonian parameters for the 1.4-eV BE. Spin-1 basis states were used in this analysis, and the (ligand) hyperfine interaction of the strength $\sim(1.3\pm0.2)\times10^{-6}$ eV was included.

g_x	g_y	g_z[a]	D_x	D_y (10^{-5} eV)	D_z[a]
1.97±0.05	1.97±0.05	2.00±0.05	−0.78±0.10	−0.78±0.10	1.56±0.10

[a]Where z‖⟨111⟩.

data a basis set of spin-1 states was used to represent the bound exciton in its triplet-spin state. All terms in Eq. (1) were diagonalized simultaneously, and the parameters obtained for best fit are given in Table I. In the fitting procedure a computer program is used for minimizing the mean-square deviation between the calculated resonance patterns and the experimental ODMR spectra. The $\underline{\mathbf{g}}$ tensor is nearly isotropic (within the experimental error). The $\underline{\mathbf{D}}$ tensor is strongly anisotropic, and both $\underline{\mathbf{g}}$ and $\underline{\mathbf{D}}$ tensors are diagonalized with the same principal axes. It is concluded from the symmetry properties of these tensors, as well as from an inspection of the anisotropy patterns in Fig. 4, that the defect has a C_{3v} point-group symmetry, i.e., the defect is axial with the defect axis along ⟨111⟩.

During the analysis, it was noticed that no satisfactory fit could be obtained unless the hyperfine interactions are included, though no hf structure was resolved in the ODMR spectra. The observed ODMR line shape could not be explained as due to the central hyperfine-interaction-induced broadening, however, it rather agrees with a hyperfine-interaction-induced broadening from the four ligand P atoms ($I_i=\frac{1}{2}$) surrounding a C_{Ga} ($I=0$) of the size $\sim1.3\times10^{-6}$ eV. It is this rather strong hf interaction that is responsible for the strong mixing of the triplet substates. Independent evidence from the study of level-anticrossing (LAC) effects for this defect confirms this strong mixing of the triplet substates.[15,16] The observation of a LAC (repulsion between approaching levels) is in fact direct proof of the presence of sizable hf interactions which induce interlevel coupling for the triplet substates. Other nuclear-electronic interactions (such as lattice distortions and vibrations, random strains, etc.) are believed to be less important in this case, since the ODMR linewidth was observed to be insensitive to crystal imperfections and external stresses.

IV. DISCUSSION

A. Electronic structure of the Cu-C defect BE

The triplet configuration of the lowest BE state studied here is a very common case for the electronic structure of neutral complex defects in GaP, which have a diamagnetic ground state when no electronic particles are bound.[5,7,10–13,17–22] It arises from an electron-hole pair (BE) bound to a defect with a low-symmetry potential, with the result that both electron and hole behave as spinlike particles. This means that the hole orbital angular momentum is quenched, which happens when the bound hole has an orbitally nondegenerate state at lowest energy.[22] This in turn normally requires a rather localized bound hole, so that the influence of the local strain field from the low-symmetry defect is strong.

The localization of the hole in this case is believed to be due to the involvement of Cu_{Ga} as part of the (Cu-C)-related defect. Cu_{Ga} is known to be a deep acceptor in GaP,[23,24] and as part of a complex defect it would create a strongly hole-attractive part of the defect potential, as also demonstrated previously for other Cu-related defects in GaP.[5,7,10–13,17–19] If this potential is rather isolated at one site of the defect, it is quite strong, and the spinlike character of the bound hole would be rather complete, leading to an essentially isotropic value for the hole $\underline{\mathbf{g}}$ tensor, $g_h\approx2.0$. The possible small anisotropy of the bound-hole $\underline{\mathbf{g}}$ tensor might be induced by the residual spin-orbit interaction on the bound hole.[22] A bound electron has so far always been observed to have an isotropic $\underline{\mathbf{g}}$ tensor ($\underline{\mathbf{g}}_e$) for various complex defects in GaP.[20,21] The $\underline{\mathbf{g}}$ tensor experimentally observed in this work is the total $\underline{\mathbf{g}}_{ex}$ tensor for the bound electron-hole pair, which in this case can simply be written as $\underline{\mathbf{g}}_{ex}=(\underline{\mathbf{g}}_e+\underline{\mathbf{g}}_h)/2$.[14] The nearly isotropic $\underline{\mathbf{g}}_{ex}$ observed, compared, e.g., to the deep Cu_{Ga}-P_{Ga} defect in GaP,[13] is consistent with only a moderately strong compensation of the donorlike and acceptorlike local potentials and a quite strong local strain field expected when an interstitial atom is part of the defect. A strong local strain field will cause a large splitting of the bound-hole states.

The Cu_{Ga} is expected to be a double acceptor. It then requires a compensation by a double donor or two single donors to produce an isoelectronic complex. A possible residual double donor present in the crystal might be the P_{Ga} antisite. The absence of the central hf structure for the P_{Ga}, which has shown a sizable doublet splitting corresponding to the nuclear spin $I=\frac{1}{2}$ from previous studies on the P_{Ga}-related defects,[13,21] excludes this possibility, however. The involvement of shallow donors in the defect complex (e.g., two Cu_i) generally results in relatively shallow defects, giving rise to BE recombination emission in the near-band-gap region.[17–19] The obvious deep donor in our case is then a C_{Ga}, and in addition a shallow donor such as a Cu_i is likely to be present, to form the isoelectronic complex. In previous work on Cu-related complexes in the near-band-gap region it was concluded that Cu_i was part of Cu-related complexes, together with Cu_{Ga}. Since C_{Ga} is predicted to be a deep donor in GaP, deeper than the Cu_{Ga} acceptor,[4] the overall average potential of a defect involving both Cu_{Ga} and C_{Ga} might be electron attractive. A total binding energy of 0.9 eV found for the 1.4-eV BE probably derives

mainly from C_{Ga}, since the 0.5-eV binding energy of Cu_{Ga} is expected to be substantially reduced when pairing with interstitial species (such as Cu_i) occurs.[5,7,10,17–19] It is therefore concluded that the C_{Ga} donor should be about 0.7 eV deep, from the present data, in agreement with theoretical calculations. Probably the isolated C_{Ga} donor can be still deeper, but no experimental data exist so far to definitely identify the energy of isolated C_{Ga}, unfortunately. The situation is similar in GaAs where a deep-donor state C_{Ga} at about 0.4 eV below the conduction band has recently been computed,[25] but not yet observed experimentally. The arguments why it is believed that C_{Ga} is involved at all in the defect studied in this work will be summarized below in Secs. IV B and IV C.

B. Identification of the Cu-C defect

The possible identity of the defect studied in this work has to be deduced from a combination of information from the sample preparation and from the electronic and structural properties derived from the PL and ODMR data. The sample-preparation procedure indicates that this defect is formed only in the case of an appreciable C concentration in the samples, and in addition after a Cu-diffusion process at quite high temperature, $T_D > 850\,^{\circ}C$. A variety of GaP samples doped with C or Cu only has not shown the ODMR signals discussed in this paper. It therefore appears clear that both C and Cu atoms are part of the defect.

As discussed above, the energy position of the BE emission spectrum for this defect indicates that a deep donor is involved as part of the defect. Isolated interstitial Cu (Cu_i) has not been observed in GaP, but previous investigations on Cu-related defects give evidence for the statement that interstitial Cu is a fairly shallow donor.[7,10,17–19] Therefore, it is believed that this deep donor is not Cu related, but consequently C related. An obvious candidate is then C_{Ga}, which should exist in the material. Interstitial C is also a possibility that cannot be neglected, since it was concluded to be involved in the shallow (Cu-C)-related defect with a BE at 2.238 eV.[5] That case indicates, however, that the C interstitial is a rather shallow donor in GaP, with possible positions on tetrahedral sites or bond centered.[5] Although another deep interstitial site for C may not be ruled out, it is considered most likely that the observed deep-donor state is due to C_{Ga}.

A possible geometrical model for the (Cu-C) complex defect studied in this work may be as follows. It involves C_{Ga} together with an acceptorlike partner of Cu_{Ga}, separated from the C_{Ga} atom along a $\langle 111 \rangle$ direction by a P atom in its regular lattice position, and in addition a Cu_i. The interstitial Cu atom is expected to be along the same axis ($\langle 111 \rangle$), in order to satisfy the C_{3v} point-group symmetry, but its position cannot be determined unambiguously from the data. If this configuration is the correct one, the donorlike and acceptorlike parts of the defect are rather well separated (third-nearest neighbors), to allow for rather strong binding of both particles, as suggested by the large total binding energy observed for the BE. It should be admitted, however, that this model is only tentative, and other configurations involving C and Cu atoms are possible. This is due to the high complexity of a three-atomic defect, which cannot be fully determined from the otherwise accurate ODMR data, in the absence of resolved hyperfine structure.

C. Defect formation

The PL data taken for C-doped GaP before and after copper diffusion yield indirect information on the defect reactions taking place in the sample. Before Cu doping, the P-site carbon acceptor bound exciton is observed with a no-phonon line at 2.322 eV.[26] This spectrum is also present in the Cu co-doped samples, but is of considerably lower intensity. The 2.238-eV BE appears after high-temperature Cu diffusion. For further increase in the diffusion temperature ($T_D > 850\,^{\circ}C$), the latter emission gradually disappears and is replaced by an infrared emission with maximum at ~ 1.4 eV. The optimum temperatures for observation of these two BE PL spectra are 850 °C for the 2.238-eV emissions and 1050 °C for the 1.4-eV emissions, respectively.

The high diffusion temperature necessary to create these two (Cu-C)-related defects must be connected with the defect reactions required to substitute first copper and then (for the 1.4-eV BE) carbon, both on Ga sites. A whole range of Cu- and (Cu-Li)-related neutral complexes was observed in our previous studies.[7,10–13,17–19] All of them, as, e.g., the (2.1774-eV) BE emission in GaP,[7] are believed to involve the Ga site substitutional copper as a part of the defect. These defects have been produced by diffusing copper into GaP at typically 900–1100 °C temperature. We may expect, therefore, that the high temperature necessary to create the 2.238-eV BE defect reflects the temperature required to substitute copper on Ga site. Carbon interstitials, believed to participate in the creation of this defect, are probably mobile at lower temperatures. The latter is assumed on the basis of the annealing studies of radiation-damaged GaP.[27–29] It has been shown that gallium and phosphorus interstitials displace carbon from the P site into interstitial sites at about 300 K. Hence, the interstitial carbon, even if not present in the starting material, may easily be created at the high temperatures used to diffuse copper. Some of these interstitial carbon donors can be stabilized when trapped at Cu_{Ga} acceptors, which we believe results in the formation of the 2.238-eV BE complex defect.[5]

The gradual disappearance of the 2.238-eV BE defect for diffusion temperatures higher than 850 °C suggests that interstitial carbon can now substitute on Ga site. A high annealing temperature (in the range of 1000 °C) and then a rapid sample quenching to room temperature are necessary to get efficient 1.4-eV BE emission, i.e., to introduce and stabilize carbon on Ga site. The Cu interstitials remain at the defect during this procedure, as indicated by the high Cu-diffusion temperatures necessary to produce the COL defect, containing Cu_{Ga} and Cu interstitials.[7]

V. SUMMARY AND CONCLUSIONS

A study of optical spectra including ODMR is reported for GaP co-doped with both Cu and C. A deep PL

spectrum with a no-phonon line at about 1.45 eV correlates with the presence of both Cu and C in the samples. This emission is shown to originate from recombination of a bound exciton with a triplet configuration as the lowest excited state. The symmetry of the defect is determined as C_{3v} from the angular dependence of the ODMR signals, and quite accurate values are derived for both **g**- and **D**-tensor parameters, from a computer fit of the spin-triplet spin Hamiltonian to the data, taking into account sizable off-diagonal interlevel couplings induced by hyperfine interactions.

It is concluded that the defect binds both the electron and the hole rather deeply, and it is argued that the electron is bound stronger. The broadening of all ODMR lines ($\sim$600 G) is consistent with ligand hf interactions with neighboring P atoms for an electron bound to a deep C_{Ga} donor. The above analysis gives rise to a tentative geometrical model of the axial defect as a row of C_{Ga}—P_P—Cu_{Ga} along a $\langle 111 \rangle$ axis, with an additional Cu_i along the same axis. The high temperature needed ($\sim$1000 °C) to produce this defect is believed to reflect the high enthalpy for substituting C on a Ga site, while at lower diffusion temperatures ($\sim$800 °C) C probably only exists on P sites and interstitial sites.

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*Permanent address: Institute of Physics, Polish Academy of Sciences, aleja Lotników 32/46, PL-02-668 Warsaw, Poland.

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