

1999

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Publication Details

This article was originally published as Heron, RJ, Lewis, RA, Simmonds, PE, Starrett, RP, Skougarevsky, AV, Clark, RG and Stanley, CR, Central-cell corrections for Si and S in GaAs in a strong magnetic field, *Journal of Applied Physics*, 85(2), 1999, 893-896. Copyright American Institute of Physics 1999. Original journal article available "[">here](#)"

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Central-cell corrections for Si and S in GaAs in a strong magnetic field

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(Received 15 June 1998; accepted for publication 12 September 1998)

The central-cell correction has been determined experimentally for the two donor impurities S and Si in GaAs. Data have been obtained for magnetic fields to 39 T, corresponding to $\gamma \approx 6$. The observed behavior is in good agreement with theory. The analysis permits accurate evaluation of zero-field central-cell corrections, yielding 0.110 and 0.059 meV for S and Si, respectively.

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I. INTRODUCTION

The electrical and optical properties of GaAs that lead to its technological importance depend in a large part on the impurities it contains, either deliberately or unintentionally introduced. Shallow donors, especially Si, are of continuing interest.¹⁻³ The usual framework for understanding the energy states of shallow donors is the effective-mass approximation which leads to a hydrogen-like energy spectrum. This article examines as a function of magnetic field one correction that needs to be applied to the hydrogenic model to fit the observed spectra, that due to the chemical identity of the donor.

In applying the hydrogenic model to *n*-GaAs, it is necessary first to scale the hydrogen energy levels by the appropriate materials parameters. The dielectric constant of GaAs, $\epsilon = 12.56$, and the effective mass of GaAs conduction electrons, $m^* = 0.0665m_e$, yield an effective Rydberg of $Ry^* = 5.72$ meV. Likewise, the dimensionless magnetic field $\gamma \equiv \frac{1}{2}\hbar\omega_c/Ry^*$, where $\omega_c = eB/m^*$, has a value of unity in *n*-GaAs for magnetic field $B = 6.57$ T; this defines an "intermediate" magnetic field. Second, additional factors, not applicable in the case of hydrogen, need to be introduced. These include band nonparabolicity,^{4,5} band anisotropy,^{4,6} and polaron effects.⁷ These effects become more pronounced as the energy of the states increases.

An unavoidable correction to the simple hydrogenic model is the central-cell correction. This arises due to differing potentials at the impurity site. This perturbation is present even in the absence of a magnetic field. Zero-field central-cell corrections have been extensively studied with a view to identifying the different chemical species involved.⁸⁻¹⁴ Compared to this large amount of work on the zero-field case, the magnetic-field dependence of the central-cell correction has been subject to little study. An early report gave the difference in chemical shift for two unidentified donors.¹⁵ Other works have used this data¹¹ or simply a

B^2 dependence¹⁶ to model the effect. These reports are limited to fields below 7 T. Even less data are available at high magnetic fields. While measurements on *n*-GaAs have been reported to 150 T, the analysis has revealed only nonparabolicity and anisotropy, and not central-cell effects.¹⁷ Unidentified donors in InSb have been studied to 20 T ($\gamma \approx 130$).¹⁸ In contrast to that study, the present article deals with the behavior of two known donors in the technologically important material GaAs. It might be noted that, apart from its inherent interest, the magnetic-field dependence of the central-cell correction permits a means for a more accurate evaluation of the zero-field effect, in that a number of data, taken at various fields, can be fitted by the theory to yield the zero-field result.

Polaron effects, which become significant at energies approaching those of the optical phonons of the host lattice, and band nonparabolicity, the effects of which increase with energy, confuse the measurement of central-cell corrections in higher-energy transitions, e.g., $1s \rightarrow 2p_0$ and $1s \rightarrow 2p_{+1}$. To minimize these effects the hydrogenic transition of lowest energy, $1s \rightarrow 2p_{-1}$, is studied here. Values for central-cell corrections derived from this transition have not been reported previously.

II. THEORY

The energy levels of the hydrogen atom in an arbitrary magnetic field are of inherent theoretical interest as well as in condensed matter physics. The area has been reviewed by Garstang.¹⁹ Very accurate calculations have been reported by Rösner *et al.*²⁰ The results of Makado and McGill²¹ include energies for a large number of states at a large number of magnetic fields. The uncertainty in these calculated results is much less than that in the experimental data.

The energy levels of chemically distinct donors differ slightly due to slightly different potentials present at the impurity site. The observed chemical shift in transition energies

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is attributed entirely to the even-parity ground state, the odd-parity final states having no chemical shift since their wave functions have zero amplitude at the impurity site. The central-cell correction takes into account the probability of finding the electron in a small volume near the impurity center. With increasing magnetic field the electron is squeezed into a smaller volume, increasing the effect. Fetterman *et al.*¹⁵ have pointed out that, using lowest order perturbation theory, the central-cell correction for a donor of species j may be written as

$$\Delta E_j = \kappa_j |\Phi(0)|^2. \quad (1)$$

Here κ_j is a constant which depends on the particular donor species and $\Phi(\mathbf{r})$ is the appropriate envelope function appearing in the effective-mass wave function of the hydrogenic ground state. According to Eq. (1), all donor species show the same relative change in ΔE_j as magnetic field, and so $|\Phi(0)|^2$ varies. Values of $|\Phi(0)|^2$ have been calculated and tabulated for a wide range of magnetic fields by Cabib, Fabri, and Fiorio.²²

III. EXPERIMENT

The high magnetic fields employed in this investigation were generated at the Australian National Pulsed Magnet Laboratory, a full description of which is given elsewhere.²³ In brief, a 32 μF capacitor bank, charged to as much as 7 kV, is discharged through a liquid nitrogen-cooled copper–silver coil. The magnetic field rises to its peak in ≈ 10 ms. Fields in excess of 60 T may be produced.

The far-infrared source is a molecular-gas cavity pumped by a CO_2 laser.²⁴ The radiation is conducted via light pipes and a top-loading probe²⁵ to the magnet bore, where the sample is located in a ^3He space. Sample temperatures below 400 mK may be maintained in this cryostat during laser irradiation. The sample mount incorporates a pick-up coil to monitor the magnetic field rise and fall and a ruthenium–oxide thermometer. Further details of the far-infrared magnetospectroscopy methods are given elsewhere.²⁶

The high-purity sample (B54) used in this investigation is a 15 μm layer grown on semi-insulating (100) GaAs by molecular-beam epitaxy, exhibiting peak mobility of $>4 \times 10^5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ in the temperature range 28–42 K. Details of the growth conditions and electrical characterization of the sample are given elsewhere.²⁷ Electrical contacts to the sample were made either by pressing indium dots onto the sample surface and annealing in a reducing atmosphere or by vacuum deposition of a Au/Ge/Ni alloy. Both types of contact gave equally satisfactory photoconductivity data.

IV. RESULTS AND DISCUSSION

The low-temperature far-infrared photoconductivity spectrum of n -GaAs is very rich in detail. The transitions of chief interest, $1s \rightarrow 2p_{-1}$, track through features of several different origins as the photon energy increases—cyclotron resonance, D^- transitions,²⁸ and transitions from the $1s$ ground state to metastable excited states.²⁹

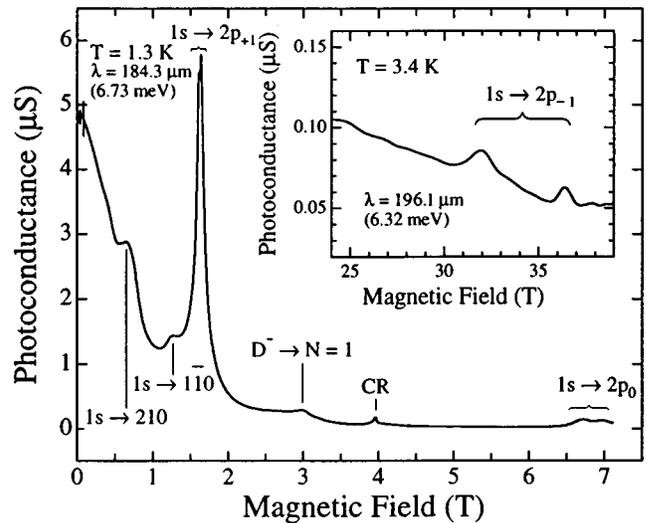


FIG. 1. Detail of photoconductivity spectra for n -GaAs. The main figure shows transitions associated with cyclotron resonance, D^- , hydrogenic bound states ($1s \rightarrow 2p_{+1}$, $1s \rightarrow 2p_0$), and metastable states [$1s \rightarrow (210)$, $1s \rightarrow (1\bar{1}0)$]. The inset shows $1s \rightarrow 2p_{-1}$ transitions. The ordinate has been offset. The two peaks seen on the ($1s \rightarrow 2p_{+1}$, $2p_0$) transitions arise from chemically distinct donors, identified (Ref. 27) as S and Si.

In Fig. 1 spectra taken at excitation wavelengths of 184.3 μm (6.73 meV) and 196.1 μm (6.32 meV) are presented. The main features are transitions from the hydrogen-like $1s$ ground state. Transitions from the $1s$ to the $2p_{+1}$, $2p_0$, and $2p_{-1}$ states are seen at about 1.6, 6.5–7, and 31–37 T, respectively, in Fig. 1. While the wave vector of the far-infrared radiation is nominally parallel to the magnetic field in our apparatus, reflection in the light pipe ensures that some component of the electric-field vector of the radiation falling on the sample is parallel to the magnetic field, allowing the observation of transitions, in particular $1s \rightarrow 2p_0$, which are strictly forbidden in the Faraday configuration. Cyclotron resonance is observed at about 4 T and $D^- \rightarrow N=1$ at about 3 T. Transitions from the $1s$ to ($1\bar{1}0$) and (210) metastable states may be seen at about 1.4 and 0.6 T, respectively. At the shortest laser wavelength used, 70.5 μm (17.58 meV), transitions to states with index as high as (710) are observed.

The transitions from the $1s$ to the $2p_{+1}$, $2p_0$, and $2p_{-1}$ states all show a splitting, as may be seen in Fig. 1. The splitting is due to the presence of two chemically distinct donors, identified as S and Si,²⁷ in the sample. The $1s \rightarrow 2p_{-1}$ transition will be analyzed in detail since, occurring at lower energy than the $2p_0$ and $2p_{+1}$ transitions, it is less affected by nonparabolicity and polaron effects. Furthermore, it remains in the far-infrared to higher magnetic fields.

The difference in the experimental energy of the $1s \rightarrow 2p_{-1}$ transition and the generic energies obtained from the hydrogen calculation is shown in Fig. 2. The theoretical value of the hydrogenic energy is obtained by interpolating data between the two fields from the given mesh of calculated values²¹ that bracket the experimental magnetic field. The interpolation is done separately for each chemical species.

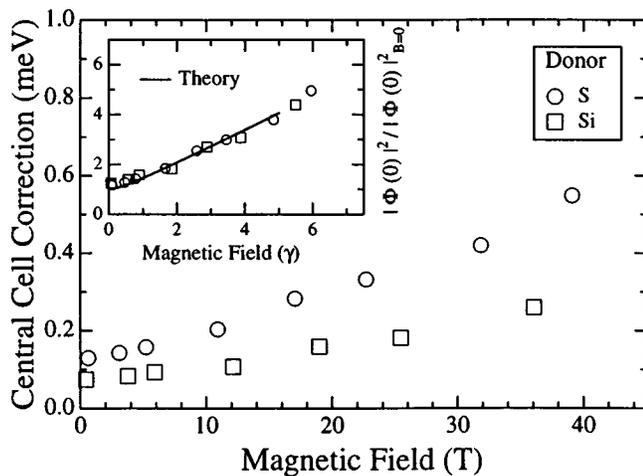


FIG. 2. Difference between experimental transition energies and energies obtained by scaling the transition energies for the hydrogen atom. Inset: Comparison of experimental data with theory Fetterman *et al.* (Ref. 15) using values of $|\Phi(0)|^2/|\Phi(0)|_{B=0}^2$ calculated by Cabib, Fabri, and Fiorio (Ref. 22).

It may be seen from Fig. 2 that, although each impurity has a different magnitude of chemical shift, both behave in a similar fashion as the magnetic field increases. The chemical effect increases with magnetic field due to the increasing magnetic confinement of the $1s$ ground state.

There is little detailed experimental data reported on the field dependence of the chemical shift. While Michels *et al.*³⁰ show line positions to 15 T, they give no values for chemical shift. Fetterman *et al.*¹⁵ give data for the difference in chemical shift for two unidentified donors, one of which is thought to have a negative central-cell correction. This data cannot be directly compared with the present results. The central-cell correction given by van Klarenbosch *et al.*¹⁴ for GaAs:Si of 0.08 meV at zero field and 0.13 meV at 6 T may be compared with the present values of 0.06 and 0.09 meV, respectively.

The inset to Fig. 2 shows the variation in central-cell correction with magnetic field according to the theoretical expression of Eq. (1) where the values of $|\Phi(0)|^2$ employed are those calculated by Cabib, Fabri, and Fiorio²² ratioed with the zero-field value of $|\Phi(0)|_{B=0}^2$. These authors give data at 16 further fields up to $\gamma=5$. These are plotted and joined to give the solid line shown.

The chemical shifts determined here by experiment are now compared directly with Eq. (1). This is accomplished by dividing the experimental fields and energies by appropriate scaling factors. The experimental magnetic fields are divided by 6.57 T to convert to units of γ . The experimental chemical shifts are divided by the central-cell correction at zero field. Rather than determine this quantity from a single, low-field measurement, the experimental data over a wide range of fields are employed. For each donor, the experimental chemical shifts are least-squares fitted to the theory values (interpolated to the experimental magnetic fields) with the zero-field central-cell correction being the fitting parameter. The zero-field central-cell corrections determined in this way are 0.110 meV for S and 0.059 meV for Si. The difference in

central-cell correction between the two species presumably reflects the difference in atomic volume, although we have not made and do not know of a detailed calculation of the size of the effect. Thus the magnetic-field dependence of the central-cell correction permits a reliable evaluation of the zero-field correction since a number of data, taken at various fields, are fitted to yield the zero-field result. Moreover, the shifts at high field are greater than the small zero-field correction, again contributing to a more reliable estimate of the latter quantity than might be made in the absence of magnetic field.

It may be seen from the inset of Fig. 2 that the field dependence of the central-cell correction as expressed in Eq. (1) following Fetterman *et al.*¹⁵ is in good agreement with the present experimental data.

V. CONCLUSION

Experimentally determined chemical shifts deduced from the $1s \rightarrow 2p_{-1}$ transition for two donors in GaAs have been given over the range $0 < \gamma < 6$.

ACKNOWLEDGMENTS

The authors thank S. Butcher, and G. Facer and B. Kane for furnishing the electrical contacts on the sample, and P. Fisher for commenting on the manuscript. This work is supported in part by the Australian Research Council, the University of Wollongong, and the University of New South Wales.

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