viated from the theoretical predictions, particularly at high fields.

(2) Three distinctive regions are observed from the I_s-versus-G plot: region I, $I_s \propto G$, $(\tau = \tau_{n0})$; region II, $I_s \propto G^{5/4}$, $(\tau \propto \Delta n^{-1/2})$, and region III, $I_s \propto G^r$, $(r = 2 \sim 2.5)$, $(\tau \propto \Delta n^{-\beta}, \beta = 1\text{–}1.5)$.

(3) The PME open-circuit voltage is found to decrease with increasing temperature as well as with decreasing photoinjection.

(4) The relative photoconductance G/G_0 has a maximum value around 20°K and decreases with either increase or decrease in temperatures.

(5) The PME apparent lifetime τ is decreased with increasing photoinjection and reaches a constant value τ_{n0} at very-high-injection levels.

(6) The high-injection electron lifetime τ_{n0} is found to decrease with decreasing temperature, indicating that the electron-capture cross section is increased with decreasing temperature.

(7) The effect of trapping in regions I and II and for $T > 20°\text{K}$ can be completely ignored, and the assumption that $\Delta_n = \Delta p$ for these two regions is experimentally verified.

(8) The effective carrier mobility is found to decrease with increasing photoinjection, which can be attributed to the increase in the ionized impurity scattering as the photoinjection is increased.

In addition, the flaw level is believed to be acceptor-type and located in the lower half of the band gap.

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Dielectric Constant of GaP at 1.6°K

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A comparison of observed and calculated line positions in a donor-acceptor pair spectrum yields a value of $\epsilon(0) = 10.75 \pm 0.1$ for the GaP static dielectric constant at 1.6°K. Earlier analyses of pair spectra assumed $\epsilon(0) = 11.1$, the value obtained from Raman-scattering measurements at 300°K. The new value of $\epsilon(0)$ necessitates a small revision in the ionization energies of some donors and acceptors.

I. INTRODUCTION

An accurate value of the static dielectric constant of GaP at room temperature, $\epsilon(0) = 11.1$, has been given by Barker,[1] who combined Raman-scattering results with an extrapolation of Bond's precise measurements[2] of the refractive index for $h\nu > 0.31$ eV. In the absence of reliable information on its temperature dependence, this dielectric constant was used for the analysis of donor-acceptor (DA) spectra measured at 1.6°K.[3,4] Now, however, we show that an accurate fitting of a pair spectrum determines a static dielectric constant of $\epsilon(0) = 10.75 \pm 0.1$ at 1.6°K.

Positive identification of the lines in a DA spectrum requires a consideration of many energy terms. Shell-structure terms depend only on the DA separation.[5] Shell-*substructure* terms depend also on the direction in the lattice from donor to acceptor.[6,7] Some energy terms arise from interactions between the neutral atoms in the *initial* state of the photon-emitting transition. Others arise from Coulomb and multipole interactions in the *final* state. A comparison of observed and calculated line positions is simplified if some of the energy terms are negligible. In this respect the best spectrum now available is that of C+O.[3,6] Our value of the dielectric constant is based on a satisfactory fitting of this spectrum.

II. FITTING C+O SPECTRUM

The C+O spectrum is particularly suitable for the determination of the dielectric constant because three

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factors contribute to its simplicity. (a) Initial-state interactions are negligible when the donor is O. (b) The V_4 multipole term is negligible when the acceptor is C, but not when the acceptor is Zn or Cd.[6] (c) Both C and O substitute on the P sublattice, so the spectrum is type I, from which the effect of the multipole term V_3 is easily removed.

The donor O has the very large ionization energy $E_D = 895.5$ meV. This implies a tightly bound electron in the neutral O, hence small polarizability. The three spectra of Ref. 3 in which the donor is O can all be fitted without van der Waals terms. The absence of a van der Waals term makes it easier to isolate the Coulomb term which we wish to use for the determination of the dielectric constant.

The complexity of a DA spectrum is largely due to the shell *substructure*, i.e., to the existence of inequivalent sets ($\langle uvw \rangle$) of sites within the same shell. The directional-energy terms are different for different sets. The characteristic doublet structure of a type-I spectrum is due to the presence of *inverse* inequivalent sets ($\pm\langle uvw \rangle$) which give rise to pairs of spectral lines that are shifted an equal but opposite amount by the odd-parity multipole term V_3.[6] Thus, the effect of V_3 can be removed from the spectrum by replacing each doublet by its center of gravity.

The analysis of the C+O spectrum can then be based on the very simple equation

$$h\nu = E_g - (E_D + E_A) + e^2/\epsilon r\,, \tag{1}$$

where $E_g = 2.339$ eV is the energy gap, E_D and E_A are the donor and acceptor ionization energies, and $e^2/\epsilon r$ is the Coulomb interaction in the final state.[8] This equation has often been used as an approximate fit to DA spectra. We are proposing to use it as an *exact* fit to the particular spectrum C+O, provided each doublet is replaced by its center of gravity.

The two parameters in Eq. (1) are the sum $E_D + E_A$ and the dielectric constant ϵ. In Fig. 1 we show an attempt to fit the data for shells $m = 5$–28, using in the bottom line the room-temperature $\epsilon = 11.1$, and the much better fit obtained in the top line by using $\epsilon = 10.75$. The experimental data in the middle line are the photon energies from Ref. 3 except that the doublets, identified in Ref. 6, are represented by their average values.[9] For some shells there is a doublet and a third line unshifted by V_3.[10] In such cases the unshifted line differs by no more than 0.2 meV from the doublet center of gravity, so it cannot be shown separately in Fig. 1.

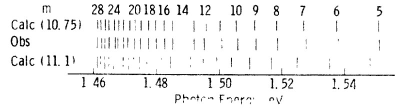

FIG. 1. Two fittings of the C+O spectrum, using $\epsilon = 11.1$ in the bottom line and the new value $\epsilon = 10.75$ at the top. The middle line gives the observed photon energies (Ref. 3) except that each doublet is replaced by its center of gravity. The values of $E_D + E_A$ used are 941.5 meV in the bottom line, 943.5 meV at the top. The shell number m is given for some lines. The absence of $m = 14$ is characteristic of the type-I spectrum.

In both top and bottom lines of Fig. 1, $E_D + E_A$ was adjusted to match the middle line at the left of the figure ($m > 20$). Only for $\epsilon = 10.75$ is the fit good throughout. Still unidentified interactions may be responsible for the remaining small misfits of order 0.5 meV, but it seems unlikely that further adjustments would affect ϵ significantly.

The most decisive lines for the determination of ϵ are those due to close pairs (small m), for which the Coulomb interaction is large. Any initial-state polarization, being attractive, would reduce the photon energy, thus reducing the Coulomb energy needed to fit the spectrum. Hence our assumption of no initial-state interaction in the C+O spectrum actually gives a lower limit for the Coulomb term, i.e., an upper limit for ϵ.

III. FITTING OTHER DA SPECTRA

The easiest DA spectrum to fit is C+O. Next easiest of those now available should be Zn+O and Cd+O,[3] for the van der Waals term is negligible when the donor is O. However, an accurate determination of the dielectric constant requires the fitting of close DA pairs, and a problem with multipole moments also arises for close pairs ($m < 10$). The V_3 and V_4 multipole terms used to fit a spectrum for large m are found to be inadequate to fit the observed lines at small m.[7] This causes no difficulty in the type-I spectrum of C+O because V_4 is negligible and V_3 is removable. However, when the acceptor is Zn or Cd, the V_4 term is no longer negligible, and V_3 is not removable from a type-II spectrum. There is no inverse relationship for the inequivalent sets of a type-II DA system. Use of $\epsilon = 10.75$ instead of 11.1 improves the fit in both the Zn+O and the Cd+O spectra, but until a satisfactory fit to the substructure is found for $m < 10$, a determination of ϵ from these spectra would have larger error limits than the ϵ found by fitting the C+O spectrum.

For most DA spectra the initial-state interactions are important. A van der Waals term accounts for most of the nondirectional part, but difficulties in fitting the multipole terms for $m < 20$ suggest that directional terms are also present.[11] Such terms are to be expected when the donor and acceptor are close enough

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[8] The DA separation r is calculated using the lattice constant $a = 5.45$ Å. The change in a between 1.6 and 300°K is about 0.1%, negligible compared with the change in ϵ; M. E. Straumanis, J.-P. Krumme, and M. Rubenstein, J. Electrochem. Soc. **114**, 640 (1967).

[9] The misfit for $\epsilon = 11.1$ was obscured in Ref. 3 by the large doublet splittings at small values of m.

[10] V_3 is zero, and there is no set inverse to $\langle uvw \rangle$ whenever one or more of u, v, or w is zero.

[11] This impediment to obtaining accurate multipole moments was not anticipated in Ref. 7.

for mutual distortion of their wave functions to occur. Thus, most DA spectra are quite unsuitable for an accurate determination of ϵ. The simplicity of the C+O spectrum is unique among those now available.

IV. TEMPERATURE DEPENDENCE OF DIELECTRIC CONSTANT

A comparison of our results with Barker's indicates a 3.3% increase, from 10.75 to 11.1, in the static dielectric constant of GaP between 1.6°K and room temperature, but direct measurements of the temperature dependence are insufficient to confirm this conclusion. The dielectric constant is the sum of electronic and lattice parts, ϵ_{el} and ϵ_{lat}, respectively, with $\epsilon_{\mathrm{el}} > \epsilon_{\mathrm{lat}}$. The contribution of the electronic part to the static dielectric constant $[\epsilon_{\mathrm{el}}(0)]$ is obtained by measuring the refractive index ($\epsilon_{\mathrm{el}} = n^2$) as a function of frequency, and then extrapolating to zero frequency. Pikhtin and Yas'kov made such measurements at 80 and 290°K.[12] They show an increase in $\epsilon_{\mathrm{el}}(0)$ of only 1.5% between 80 and 290°K, but their results depend on a fairly long extrapolation. We know of no experimental work on the temperature dependence of ϵ_{lat}.

Faulkner has determined the low-temperature values of $\epsilon(0)$ for Si and Ge by fitting the absorption spectra of shallow donors.[13] His results indicate increases of 2.5 and 4.2%, respectively, for Si and Ge between liquid-helium and room temperature. These dielectric-constant increases are consistent with the refractive-index increases measured by Cardona, Paul, and Brooks.[13]

V. IONIZATION ENERGIES

Use of the new value $\epsilon = 10.75$ in the analysis of DA spectra yields new values of $E_D + E_A$, in most cases about 2 meV higher than the values obtained with $\epsilon = 11.1$. We now find $E_D + E_A = 152$ meV for the shallow C+S pair spectrum. To split this energy between donor and acceptor we rely on Onton's value of 104 meV for the ionization energy of the donor S, obtained by analyzing the infrared excitation spectrum of S.[14] We therefore take $E_A(\mathrm{C}) = 48$ meV.[15] Combining this with the new value $E_D + E_A = 943.5$ meV for the C+O spectrum, we obtain $E_D = 895.5$ meV for the deep O donor. This value fits the photoexcitation spectrum of the O donor[16] significantly better than the lower estimate (893±2 meV) in Ref. 3.

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[15] Acceptor ionization energies derived from the pair spectra are accurate to ≈±1 meV, mainly because of the uncertainty in E_g. Relative values are accurate to better than ±0.5 meV.

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Epitaxy of CdS on SrF_2

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The epitaxy of wurtzite CdS on (111)-cleavage planes of SrF_2 is examined theoretically and experimentally. The theoretical treatment is based on the assumption that the predominent interaction across the film-substrate interface is of an ionic type. The energy of a unit of the CdS films interacting with the substrate is calculated by lattice summation as a function of position and orientation. Based on a minimum-energy criterion, the calculation shows that it is more favorable for a sulfur layer rather than a cadmium layer to be immediately adjacent to the substrate. Further, the calculation yields the positions on an atomic scale of the atoms of the deposit relative to those of the substrate. Epitaxial films of CdS on SrF_2 were grown using a chemical transport reaction and were shown to have the wurtzite structure with the [0001] direction of the deposit parallel to the [111] direction of the substrate. The $[1\bar{1}00]$ direction of the film is perpendicular to the $[10\bar{1}]$ direction of the substrate. An experimental investigation of the film surfaces using an ion-scattering method verified the prediction that a sulfur layer is immediately adjacent to the substrate.

I. INTRODUCTION

The growth of epitaxial films of CdS on (111)-cleavage planes of CaF_2 and of CdSe on (111)-cleavage planes of CaF_2 and BaF_2 has been reported in the literature.[1–4] These reports deal primarily with the crystallinity of the films and the measurement of optical and electrical properties. There is little information available on the atomic arrangement at the film-sub-

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