PHYSICAL REVIEW B VOLUME 42, NUMBER 5 15 AUGUST 1990-I

Observation of a metallic impurity band in *n*-type GaAs

D. Romero, S. Liu, and H. D. Drew
Joint Program for Advanced Electronic Materials, Department of Physics, University of Maryland, College Park, Maryland 20742
and Laboratory for Physical Sciences, College Park, Maryland 20740

K. Ploog
Max-Planck-Institut für Festkorperforschung, D-7000 Stuttgart 80, Federal Republic of Germany

(Received 21 February 1990)

Magnetotransport and far-infrared spectroscopy are combined to probe the electronic states in the vicinity of the magnetic-field-induced metal-insulator transition in *n*-type GaAs. Resonant absorption lines, identified as the shallow-donor 1*s*-2*p* transitions by their selection rules, magnetic-field dependence, and temperature dependence are observed even in the metallic state. These results demonstrate that, near the metal-insulator transition, the electrons are in the donor impurity band, which is split off from the conduction band.

Semiconductors doped above a critical density, n_c, remain conducting down to the lowest temperatures. As the carrier density is lowered through n_c or if a magnetic field greater than a critical field, B_c, is applied, a metal-insulator transition (MIT) occurs. At the MIT the extended electronic states near the Fermi level become localized. This is an example of localization in disordered systems, a topic which has received much attention and has seen much progress in recent years.[1] Despite the progress made in understanding the MIT, fundamental questions remain unanswered. For the case of doped semiconductors, the question of whether the MIT takes place in the conduction band or in the impurity band has been debated for many years. Therefore, whether an impurity band can support metallic conduction is not established. Theory has not been decisive on these issues. Estimates for the density, n_i, for which the impurity (lower Hubbard) band splits off from the conduction band, vary from $n_i \cong n_c/10$ to $n_i \cong 10n_c$.[2-4] A recent calculation for a disordered system based on a multiple-scattering approximation[4] gives $n_i \cong n_c/10$. The existing experimental data are similarly inconclusive. The literature is rife with conflicting conclusions on this question based on transport measurements.[2,5] The only far-infrared studies for $n \cong n_c$ were on Si:P in zero magnetic field.[6] In this work the distinct 1*s*-2*p* multiplets have disappeared by $n \simeq n_c/4$, but a broad absorption band remains near the average 1*s*-2*p* frequency. The leading edge of this absorption was attributed to absorption by high-density clusters of donors. In Raman studies on Si:P (Ref. 7) and Ge:As (Ref. 8), resonances, interpreted as transitions between the valley-orbit-split ground-state levels, are observed to persist to densities near (and above, for Ge:As) n_c. However, since these resonances could arise from intervalley scattering effects of carriers in the conduction band,[7,8] their implications on the issue of a metallic impurity band are not completely clear.

In an earlier paper[9] we reported the results of Faraday-geometry (photon $\mathbf{q}\|\mathbf{B}$) far-infrared magneto-optical measurements on *n*-type GaAs. $1s \rightarrow 2p^{\pm}$ donor transitions were observed and found to persist through the magnetic-field-induced MIT. Since the $1s \rightarrow 2p^{+}$ and $1s \rightarrow 2p^{-}$ resonances are broad at these impurity densities ($n \cong n_c$), they are not resolved at low magnetic fields, so it was not possible to follow them through the low-magnetic-field range. In this paper we present additional measurements that we believe make a compelling case, for the first time, for the observation of metallic impurity band. We have observed and studied the $1s \rightarrow 2p^0$ transition in the Voigt geometry ($\mathbf{q} \perp \mathbf{B}$). The selection rules, temperature dependence, and magnetic field dependence observed for this resonance, together with the earlier Faraday-geometry results, are all consistent with the observation of transitions from a 1*s* impurity band to a 2*p* impurity band on both the metal and insulator sides of the MIT.

The samples investigated in this study were (2–4)-μm-thick *n*-type GaAs (Si-doped) epitaxial layers, grown on semi-insulating GaAs substrates by molecular-beam epitaxy. dc-transport measurements were made on samples, typically 2×10 mm^2, with annealed indium contacts in a Hall-bar configuration. The carrier densities, compensations, and 77-K mobilities, after corrections due to depletion layers and the Hall scattering factor,[10] are summarized in Table I. Two of these samples (2 and 3) have carrier densities above the zero-magnetic-field critical density ($n_c \cong 1.5 \times 10^{16}$ cm^{-3}) given by the Mott MIT condition, $n_c^{1/3} a^* = 0.25$, where a^* is the donor effective Bohr radius. The longitudinal magnetoresistance was measured for these samples for temperatures $T \geq 0.45$ K and magnetic fields $B \leq 9$ T. Far-infrared magnetotransmission was measured in the Voigt geometry for magnetic fields up to 11 T and temperatures ranging from 2 to 50 K using a SPECAC Fourier-transform spectrometer. The sample probe is equipped with an externally controlled linear polarizer, which permits the study of

TABLE I. Sample parameters.

Sample no.	$n=N_d-N_a$ (cm^{-3})	$K=N_a/N_d$	μ_H (cm^2/V s)	B_c (T)	B_{SdH}[a] (T)
1	1.30×10^{16}	0.18	21 000		
2	3.50×10^{16}	0.27	10 000	4.9	2.4
3	5.60×10^{16}	0.27	8 900	7.5	2.8

[a] SdH denotes Shubnikov–de Haas.

the transmission in both the **E**‖**B** and **E**⊥**B** polarizations, and a two-position sample holder, which can also be switched from the outside. The measured quantity was the ratio of the transmission of the sample to that of a reference semi-insulating GaAs substrate.

At low temperatures the longitudinal resistance of samples 2 and 3 displays a negative magnetoresistance at low field, followed by a single Shubnikov–de Haas (SdH) oscillation, and then a large and strongly-temperature-dependent increase in the resistance and Hall coefficient at higher magnetic fields. These features have been observed previously in GaAs.[11] The high-field behavior is characteristic of the transition from the metallic to the insulating state. The best estimate for the critical field, B_c, for the metal-insulator transition can be obtained by extrapolating the temperature dependence of the longitudinal conductivity, $\sigma_L(T)$, to $T=0$ K. The magnetic field where $\sigma_L(0)=0$ gives the value of B_c.

At finite temperatures corrections to the Boltzmann conductivity, due to disorder and electron-electron interaction, have been calculated and verified experimentally for different conducting systems in the weakly localized regime.[1,12] In three dimensions, elastic scattering gives rise to a "weak-localization" correction associated with interference of backscattered waves. At finite temperature, inelastic scattering cuts off the interference, giving rise to a $\delta\sigma(T)\propto T$ conductivity term. Electron-electron interactions give a $\delta\sigma_L(T)\propto T^{1/2}$ correction.[13] The interference effect is quenched at high magnetic fields, and the temperature dependence of the conductivity is determined by the interaction effects only. At sufficiently low temperature, i.e., $\pi k_B T < |\mu g B|$, spin-orbit scattering changes the interaction correction to the conductivity to a $T^{1/3}$ dependence.[14] A $T^{1/3}$ dependence, close to the MIT, was recently verified by Maliepaard *et al.*[15] in measurements on *n*-type GaAs.

A plot of $\sigma_L(T)$ versus $T^{1/3}$ for our high-density sample 3 for different values of magnetic field near B_c is shown in Fig. 1. The data are seen to approach a $T^{1/3}$ dependence for temperatures below $\simeq 1$ K. This behavior is consistent with the spin-orbit-scattering condition given above. To estimate B_c from these data, we extrapolate the $T^{1/3}$ dependence below 1 K to zero temperature, as shown in the figure. It can be seen from Fig. 1 that $B_c \approx 7.5\pm0.1$ T. These data were also analyzed assuming a $T^{1/2}$ dependence below 1 K, and this results in a 4% increase in the estimated B_c. In this case, however, the fit below 1 K is not as good. For sample 2 the spin-orbit-scattering condition for magnetic fields near the MIT ($\cong 5$ T) corresponds to temperatures below $\cong 0.6$ K. Therefore our estimate of B_c for this sample must be more indirect, and therefore less precise. We note, as reported earlier,[9] that in the range $0.5 \le T \le 4$ K σ_L is found to vary as $T^{1/2}$ for this sample. Extrapolating this dependence gives $B_c = 5.3$ T.[9] This is probably an upper limit for B_c, however, since σ_L is expected to bend over at $T \cong |\mu g B|/\pi k_B$, as observed in our higher-density sample (Fig. 1) and in the data reported by Maliepaard *et al.* on a lower-density sample.[11] A lower limit for B_c for sample 2 is given by the Shubnikov–de Haas oscillation observed at 2.4 T. If we interpolate both the low- and high-temperature behavior of σ_L between our high-density sample and the low-density sample of Maliepaard *et al.*, we obtain $B_c = 4.9\pm0.4$ T for sample 2. We emphasize that precision in the determination of B_c is not critical for the major conclusions of this work.

Typical far-infrared transmission spectra for sample 2 in the **E**‖**B** polarization are shown in Fig. 2. A single broad absorption line is observed which shifts towards higher energy and narrows as the magnetic field is increased. The observed resonance positions for three of the samples that we have investigated are shown in Fig. 3. The resonance frequencies are seen to be close to, but shifted below, the frequency of the $1s$-$2p^0$ transition for

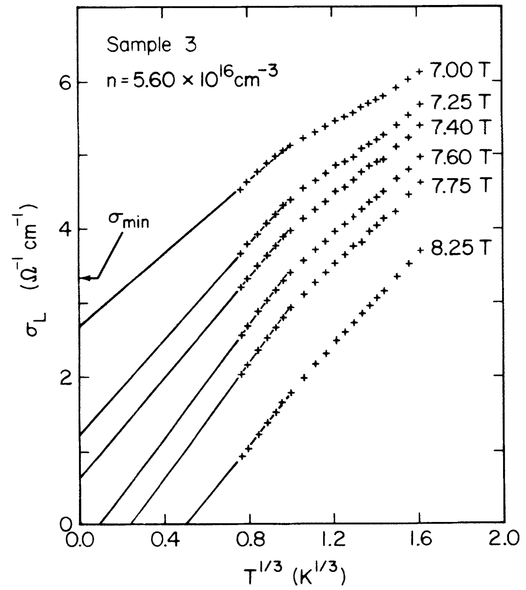

FIG. 1. Plot of the longitudinal conductivity $\sigma_L(T)$ vs $T^{1/3}$ for sample 3 for different magnetic fields near the MIT. The crosses are experimental data and the solid curves represent the extrapolations to 0 K. The position of the Mott minimum metallic conductivity (Ref. 2) is indicated in the figure.

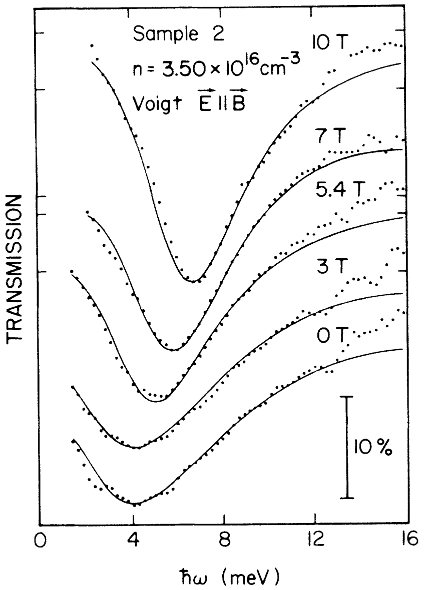

FIG. 2. Far-infrared transmission of sample 2 for different magnetic fields at 4.2 K. The dots are data points and the solid curves are line-shape fits as described in the text. The critical field for this sample is $B_c = 4.9$ T. The tic marks on the vertical axis correspond to the 50% transmission level for the given magnetic field. The 10% transmission scale is also indicated.

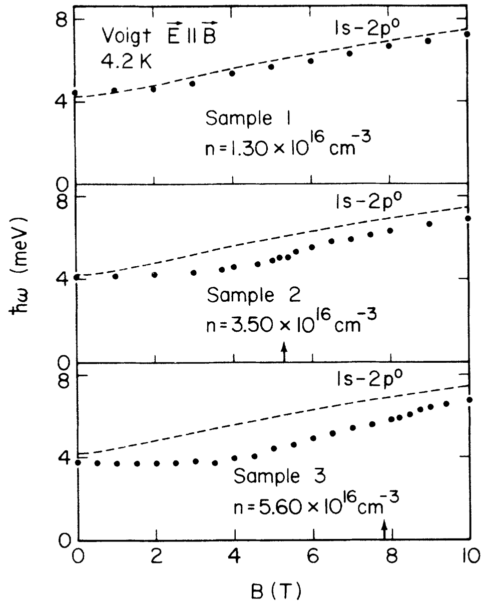

FIG. 3. Plot of the resonance-peak positions vs magnetic field for the three samples. The solid circles are the positions of the minimum point from the transmission line shapes, while the dashed curves are the theoretical values of the isolated 1s-2p^0 transition energy obtained from Larsen (Ref. 12). The arrows mark the position of the critical field for samples 2 and 3.

an isolated donor in GaAs.[16] As can be seen in Fig. 3, this shift is largest for fields $\leq B_c$ and approaches zero at $B = 0$ T, and at large fields, where the overlap of the donor wave functions is reduced. In the Voigt **E**⊥**B** geometry we observe two peaks, corresponding to the 1s-2$p^{\pm}$ transitions, confirming the Faraday results. We emphasize that all these resonances are consistent with the selection rules of the 1s-2p transitions and that they are observed on both the metallic and insulating sides of the MIT.

It is the temperature dependence of these spectra that provide the strongest evidence of the split-off impurity band on the metallic side of the MIT. In Faraday geometry, at $B = 4$ T, where sample 2 is metallic, the 1s-2$p^{\pm}$ resonance at 4.2 K is replaced by cyclotron resonance for $T \gtrsim 40$ K. In Voigt **E**∥**B** geometry at $B = 2.4$ T, the oscillator strength of the 1s-2p^0 resonance peak that we observed at 4.2 K reduces as the temperature is increased and becomes unobservable for $T \geq 40$ K. As the 1s-2p^0 resonance weakens, its oscillator strength is replaced by a free-carrier-like absorption, as shown in Fig. 4.

We have analyzed these transmission spectra using a model dielectric function,

$$\epsilon = \epsilon_0 + \frac{\omega_p^2 f_0}{\omega_0^2 - \omega^2 - i\omega\Gamma_0} + \frac{\omega_p^2 f_d}{\omega(\omega - i\Gamma)} ,$$

where ω_0 is the resonance-peak position, the f's represent the oscillator strengths, the Γ's are linewidths, $\omega_p = 4\pi n e^2/m^*$ is the plasma frequency with n taken as the measured Hall density, and ϵ_0 is the static lattice dielectric constant of GaAs. The second term is a bound-state Lorentzian oscillator to model the 1s-2p^0 absorption. The third term represents a Drude contribution corresponding either to the response of the conduction-band electrons (cyclotron resonance is not excited in the **E**∥**B** geometry) or to intra-impurity-band ab-

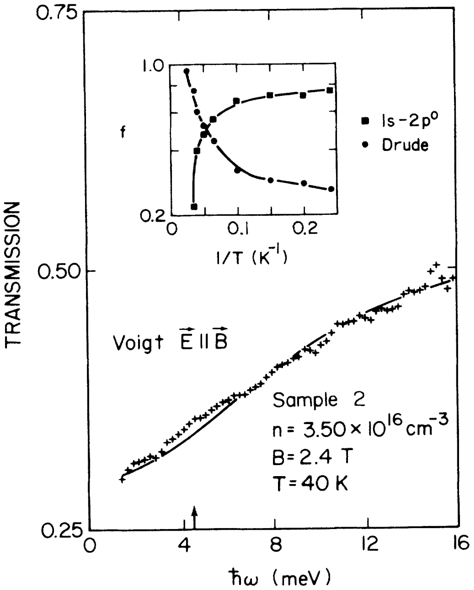

FIG. 4. Transmission spectrum at 40 K and 2.4 T for sample 2 in the Voigt **E**∥**B** geometry. The solid curve is a least-squares fit to the data (crosses) obtained from the transmission calculated from the model dielectric function described in the text. The arrow marks the position of the 1s-2p^0 transition for this field. The inset is an Arrhenius plot of the oscillator strengths obtained from the fitting.

sorption processes. In Fig. 2 we show the least-squares fits made to the transmission data with ω_0, the Γ's, and f's as fitting parameters. ω_0 is found to be close to the minimum of the absorption spectra, and the sum of the oscillator strengths, f_0+f_d, is found to be constant and $\cong 1$ for all T and all B, showing that all of the carriers are accounted for. The success of the line-shape analysis gives further credence to the impurity-band interpretation of these data.[17]

The oscillator strengths of the $1s$-$2p^0$ transition and the Drude-type absorption for sample 2, derived from the line-shape analysis at $B=2.4$ T (where the sample is metallic), is shown in an Arrhenius plot in the inset of Fig. 4. In the low-temperature range ($T \leq 10$ K) f_d (the Drude term) becomes important only at low fields, when the samples are metallic. This term is needed to fit the low-frequency transmission. It implies either an intra-impurity-band absorption process or transitions from the upper Hubbard band to the conduction band. From the high-temperature behavior of the oscillator strengths, we estimate an activation energy of $E_a \approx 1.9$ meV, which is less than the binding energy of an isolated donor in GaAs. This activation energy is found to increase with magnetic field, $E_a \cong 2.6$ meV at 5.3 T and 3.4 meV at 8 T. These results imply the thermal excitation of the electrons from the impurity band to the conduction band, even on the metallic side of the MIT.

In measurements on an $n=9.7\times10^{16}$ cm^{-3} sample, there is no evidence for the $1s$-$2p$ transition at $B=0$ T. The spectra can be described with a pure Drude response function. From this observation we conclude that the impurity band merges with the conduction band for $n_i \simeq 8\times10^{16}$ cm$^{-3} \simeq 5n_c$. Another interesting conclusion of this work is that the Shubnikov–de Haas bump observed in the transport must be associated with carrier transport in a metallic impurity band.

ACKNOWLEDGMENTS

We thank M. Shayegan and B. Elman for providing samples in the early phases of this work. We acknowledge useful discussions with D. Belitz, S. Das Sarma, D. Larsen, M. W. Lee, and R. E. Prange. The work was supported, in part, by the U.S. National Science Foundation, Under Grant No. DMR-87-0-4670 and by the U.S. Office of Naval Research, under Grant No. N00014-89-J-1551.

---

[1] For a recent review, see B. L. Al'tshuler and P. A. Lee, Phys. Today **41**(12), 36 (1988).

[2] N. F. Mott and E. A. Davis, *Electronic Processes in Non-Crystalline Solids* (Oxford University Press, London, 1979), Chap. 4.

[3] K. A. Chao, R. Rikland, and A. Ferreira da Silva, Phys. Rev. B **21**, 5745 (1980); J. H. Rose, H. B. Shore, and L. M. Sander, *ibid.* **21**, 3037 (1980); R. N. Bhatt and T. M. Rice, *ibid.* **23**, 1920 (1981).

[4] J. Serre and A. Ghazali, Phys. Rev. B **28**, 4704 (1983).

[5] See, e.g., *Proceedings of the International Conference on Localization, Interaction, and Transport Phenomena,* edited by G. Bergmann and Y. Bruynseraede (Springer-Verlag, New York, 1985), and literature cited therein.

[6] G. A. Thomas, M. Capizzi, F. DeRosa, R. N. Bhatt, and T. M. Rice, Phys. Rev. B **23**, 5472 (1980).

[7] K. Jain, S. Lai, and M. Klein, Phys. Rev. B **13**, 5448 (1976).

[8] J. Doehler, P. J. Colwell, and S. A. Solin, Phys. Rev. Lett. **34**, 584 (1975).

[9] D. Romero, Ming-Way Lee, H. D. Drew, M. Shayegan, and B. S. Elmanin, in *Proceedings of the International Symposium on Anderson Localization,* edited by T. Ando and H. Fukuyama (Springer-Verlag, New York, 1987); Ming-way Lee, D. Romero, H. D. Drew, M. Shayegan, and B. S. Elman, Solid State Commun. **66**, 23 (1988).

[10] A. Chandra, C. Wood, D. Woodward, and L. Eastman, Solid-State Electron. **22**, 645 (1979); R. K. Willardson and A. C. Beer, *Semiconductors and Semimetals 10* (Academic, New York, 1980), p. 71; B. R. Nag, *Electron Transport in Compound Semiconductors* (Springer-Verlag, Berlin, 1980), p. 380.

[11] See, e.g., M. C. Maliepaard, M. Pepper, R. Newbury, J. E. F. Frost, D. C. Peacock, D. A. Ritchie, G. A. C. Jones, and G. Hill, Phys. Rev. B **39**, 1430 (1989), and references cited.

[12] For additional reviews, see N. F. Mott and M. Kaveh, Adv. Phys. **34**, 329 (1985); P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).

[13] See, e.g., H. Fukuyama, in *Electron-electron Interactions in Disordered Systems,* edited by A. L. Efros and M. Pollak (Elsevier, Amsterdam, 1985).

[14] A. M. Finkel'shtein, Pis'ma Zh. Eksp. Teor. Fiz. **37**, 436 (1983) [JETP Lett. **37**, 516 (1983)].

[15] M. C. Maliepaard, M. Pepper, R. Newbury, and G. Hill, Phys. Rev. Lett. **61**, 369 (1988).

[16] The theoretical curve for isolated donors, shown in Fig. 3, and which is in excellent agreement with the experimental data on high-purity n-type GaAs, was provided by D. Larsen (private communication).

[17] Attempts to fit the spectra to a model consisting of (statistically) isolated donors embedded in a metallic matrix using effective-medium theory for the dielectric function gave clearly poorer results.