

Metal-insulator transition in the compensated semiconductor Si:(P,B)

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The results of a continuing investigation of the effects of impurity compensation on the characteristics of the metal-insulator ($M-I$) transition in Si:P are reported. The system used is Si:(P,B). Most of the information is derived from measurements and analysis of the dc electrical conductivity σ in the temperature range $50 \text{ mK} < T < 4 \text{ K}$. The form of the temperature dependence of σ in this range is extensively studied. For samples with electron concentration n near n_c , the critical concentration for the $M-I$ transition, the temperature dependence of σ departs significantly from the form $\sigma = \sigma(0) + mT^{1/2} + BT^{3/4}$, which describes samples at higher values of n . As K , the ratio of acceptor to donor concentration, is increased from zero, the value of n_c first decreases slightly before rising sharply at larger values of K . Measurements of $\sigma(0)$ as a function of n in uncompensated Si:P agree with data in the literature. The applicability of the scaling theory to a description of our measurements of $\sigma(0)$ as a function of n in compensated samples is questioned. Attention is given to establishing the most reliable methods for determining values of impurity concentrations.

I. INTRODUCTION AND OVERVIEW

In a previous publication¹ (which we shall designate as HTH), we reported measurements of the dc electrical conductivity of the compensated semiconductor Si:(P,B) near the metal-insulator ($M-I$) transition. The data were interpreted in terms of the scaling theory of localization.² The present paper represents an extension of that earlier study in several directions.

(1) In HTH, two sets of samples with carrier concentration n near the critical concentration n_c were investigated, one set with compensation ratio $K \equiv N_B/N_P = 0.24$ to 0.43 ($K_c = 0.43$) and the second with $K = 0.34$ to 0.52 ($K_c = 0.52$). N_P and N_B are the phosphorus and boron concentrations, respectively, and K_c is the value of K at $n = n_c$. Significant differences from the behavior of the reference system Si:P ($K = 0$) were observed. In the present work, we add measurements on a set of samples of lower compensation, with $K = 0.2$. Data from this additional set of samples, plus further investigation of the most reliable methods of determining impurity concentrations, give us important information about the dependence of n_c on the compensation ratio K . We report small adjustments in values of K for samples referenced in HTH. We find, surprisingly, that the value of n_c at $K = 0.2$ is slightly lower than the value for uncompensated Si:P. For larger amounts of compensation ($K > 0.4$), n_c does increase sharply, in response to the increasing fluctuations in impurity potentials in the more heavily compensated samples. Shklovskii and Efros³ have presented a calculation of the effects of those increased fluctuations. Their results are, however, only applicable for high compensation, with the value of K near unity.

We include results of measurements made in our laboratory on a set of samples with $K = 0$. These measurements were made to make certain that our results are

properly linked to the extensive earlier work on Si:P.⁴

(2) For compensated samples with n far into the metallic region, the temperature dependence of the conductivity below 4 K is well described by the form previously used in HTH,

$$\sigma = \sigma(0) + mT^{1/2} + BT^{3/4} . \quad (1)$$

For compensated samples in the "just-metallic" regime ($1 < n/n_c < 1.1$), we find the temperature dependence of σ at low T to depart significantly from Eq. (1). Consequently the values of $\sigma(0)$ extracted from fits of Eq. (1) for samples with $n/n_c < 1.1$ are overestimates. A modified form of Eq. (1), with the exponent $\frac{3}{4}$ replaced by an adjustable parameter a , such that

$$\sigma = \sigma(0) + mT^{1/2} + BT^a , \quad (2)$$

gives an improved fit to the low-temperature data. We may here be seeing the shift in temperature dependence of the localization term from $T^{3/4}$ to $T^{1/2}$ which has been calculated by Isawa.⁵ As n approaches n_c the changing temperature dependence makes any extrapolation procedure to obtain $\sigma(0)$ increasingly suspect. Experimental distinction between metallic and insulating behavior becomes increasingly difficult.

As n approaches n_c and T approaches 0, small inhomogeneities in our samples as well as samples used by others may obscure the true behavior of $\sigma(T)$. Such inhomogeneities can arise in the Czochralski growth process. We cannot exclude the possibility that in fully homogeneous samples $\sigma(0)$ drops to zero discontinuously at n_c . It is our guess that this problem might be affecting all values of $\sigma(0)$ which are less than $20 \Omega^{-1} \text{ cm}^{-1}$, the value of σ_{min} for Si:P.

(3) If we use the scaling theory² expression for $\sigma(0)$ as a function of n ,

$$\sigma(0) = \sigma_0 \left(\frac{n}{n_c} - 1 \right)^\mu, \quad (3)$$

we find that the value of μ for our samples with $K=0.2$ depends strongly on our method of analysis. Using the values of $\sigma(0)$ which were obtained from fits of Eq. (1), we find $\mu=0.9$. Using improved estimates of $\sigma(0)$ resulting from fits of Eq. (2), we find $\mu=0.5$. Interestingly, the values 0.5 and 0.9 are the limiting values previously found for uncompensated Si:P⁴ and heavily compensated Si:(P,B),¹ respectively. Obviously, our analysis cannot distinguish definitively between those two values of μ for this set of samples.

It is important to note that an equally good fit to the data for the more heavily compensated samples ($K_c=0.45$ and $K_c=0.6$) can be obtained using a Boltzmann form for the conductivity as modified by weak localization corrections,⁶

$$\sigma(0) = \sigma_B \left[1 - \frac{3}{(k_F l)^2} \right], \quad (4)$$

where $\sigma_B = ne^2 l / \hbar k_F$ is the Boltzmann conductivity, k_F is the Fermi wave vector, and l is the elastic mean-free path. For uncompensated Si:P, in contrast, the variation of $\sigma(0)$ as n approaches n_c is much steeper⁷ than predicted by Eq. (4).

The scaling theory fit is expected to be valid only in a critical region just above n_c . The weak localization fit is based on a perturbation theory approach which is expected to break down as n decreases toward n_c , and the mean-free path approaches the Ioffe-Regel⁸ limit $l_{IR} = \pi/k_F$. In the compensated samples, we can discern no clear dividing line between applicability of the two theoretical models for the behavior of $\sigma(0)$.

II. EXPERIMENTAL DETAILS

We cut our samples from four custom-grown crystals of n -type Si:(P,B) labeled *A* through *D*.⁹ Table I gives some characteristics of the samples, including measured values of the room-temperature resistivity $\rho(296 \text{ K})$ and the room-temperature Hall coefficient $R_H(296 \text{ K})$. The Czochralski growth process produces gradients in phosphorus and boron concentration along the length of each crystal. The samples are numbered according to their position along the crystal, starting at the seed end. We also obtained wafers of uncompensated Si:P.¹⁰ Four-point probe resistivity mappings on wafers with thicknesses of 250 to 380 μm were used to locate sufficiently homogeneous regions, from which we cut 8-mm-diameter cloverleaf samples. For more details about sample selection and preparation, see Refs. 1, 11, and 12.

For all of our samples, we obtained the phosphorus concentration N_P from neutron activation measurements.¹² Unfortunately, a sufficiently accurate direct determination of the boron concentration N_B for the compensated samples was not achieved. Therefore, we measured $R_H(296 \text{ K})$ in order to determine the carrier concentration n . [Procedures for extracting values of A to use in the relationships $R_H(296 \text{ K}) = A/ne$ are de-

scribed in the Appendix.] Using $n = N_P - N_B$, one can then determine N_B and $K \equiv N_B/N_P$. In Table I, we show the room-temperature characteristics of our samples together with values of the zero-temperature conductivity $\sigma(0)$ determined as discussed below. We note that because of improvements in our characterization procedures, the listed values of n and K do not agree with previously published¹ values for samples studied in HTH. See the Appendix for a more detailed description of our procedures for determining dopant and carrier concentrations.

We measured the electrical conductivity $\sigma(T)$ of most samples between 1.3 K and 4.2 K using the van der Pauw technique.¹³ For samples near the metal-insulator transition, we extended these measurements down to 50 mK. Below 50 mK, the thermal contact between our samples and thermometry was not good enough to ensure an ac-

TABLE I. Characteristics of Si:(P,B) samples. Values of n and K are obtained as described in the Appendix; values of $\sigma(0)$ are derived from fits of Eq. (1); $\rho(296 \text{ K})$ and $R_H(296 \text{ K})$ are measured directly. Values of K listed in parentheses are estimates rather than measured data. Values of $\sigma(0)$ listed in parentheses for the four lowest concentration samples of crystal *D* are derived from fits of Eq. (2) rather than Eq. (1).

| Sample | n^a (10^{18} cm^{-3}) | K^a | $R_H(296 \text{ K})$ (cm^3/C) | $\rho(296 \text{ K})$ ($\text{m}\Omega \text{ cm}$) | $\sigma(0)$ ($\Omega^{-1} \text{ cm}^{-1}$) |
|--------|--|--------|--|--|--|
| A-1 | 3.68 | 0.51 | 2.22 | 26.72 | 0 |
| A-9 | 3.75 | (0.5) | 2.18 | 24.88 | 1.3 |
| A-48 | 4.23 | (0.45) | 1.92 | 22.67 | 22.2 |
| A-87 | 4.74 | 0.46 | 1.70 | 21.09 | 36.9 |
| A-63 | 4.94 | 0.43 | 1.63 | 19.77 | 50.1 |
| A-64 | 5.03 | 0.40 | 1.60 | 20.11 | 45.9 |
| A-73 | 5.33 | 0.42 | 1.50 | 18.96 | 56.7 |
| A-77 | 5.67 | 0.39 | 1.41 | 17.74 | 69.9 |
| A-111 | 5.92 | 0.38 | 1.34 | 17.00 | 77.2 |
| A-105 | 6.67 | 0.33 | 1.18 | 15.28 | 99.7 |
| A-130 | 8.11 | 0.29 | 0.95 | 12.32 | 147 |
| A-194 | 9.66 | 0.33 | 0.78 | 10.10 | 201 |
| B-270 | 4.34 | (0.6) | 1.87 | 33.70 | 0 |
| B-265 | 4.69 | (0.6) | 1.73 | 30.21 | 6.2 |
| B-266 | 5.20 | (0.6) | 1.56 | 27.67 | 14.4 |
| B-285 | 5.33 | 0.58 | 1.50 | 27.57 | 14.9 |
| B-310 | 5.88 | 0.56 | 1.36 | 24.06 | 29.2 |
| B-312 | 6.61 | 0.54 | 1.19 | 20.90 | 53.1 |
| B-322 | 7.16 | 0.49 | 1.09 | 18.79 | 69.3 |
| B-348 | 8.26 | 0.42 | 0.93 | 15.84 | 99.0 |
| B-320 | 8.83 | 0.39 | 0.87 | 14.40 | 117 |
| B-354 | 9.15 | 0.45 | 0.83 | 14.08 | 121 |
| D-254 | 3.57 | (0.2) | 2.30 | 14.97 | 5.5 (0.0) |
| D-269 | 3.67 | (0.2) | 2.23 | 14.60 | 12.4 (4.1) |
| D-280 | 3.72 | 0.23 | 2.20 | 14.81 | 19.9 (16.5) |
| D-336 | 3.72 | 0.24 | 2.20 | 14.95 | 20.3 (19.2) |
| D-325 | 3.91 | 0.24 | 2.09 | 14.47 | 29.9 |
| D-290 | 3.93 | (0.2) | 2.08 | 14.00 | 33.7 |
| D-316 | 4.14 | (0.2) | 1.97 | 13.70 | 48.2 |
| D-317 | 4.14 | (0.2) | 1.97 | 13.25 | 50.7 |

^aValues of n and K for samples previously used in Ref. 1 have been readjusted due to improved sample characterization procedures (see Appendix).

curate measurement of the sample temperature. For some samples, only measurements below 1.3 K were performed.

III. RESULTS AND ANALYSIS

A. Temperature dependence of conductivity

The temperature dependence of the electrical conductivity at low temperature has historically been and continues to be a vital piece of information in exploring the nature of the $M-I$ transition. There are two reasons for this importance. (1) Given the experimental inability to reach $T=0$ K, extrapolation procedures are required in order to obtain values of $\sigma(0)$, a key quantity in distinguishing metal from insulator. (2) The form of $\sigma(T)$ gives valuable information about the nature of the electron transport in the nearly localized system.

Figure 1(a) displays data for $\sigma(T)$ in the 0 K to 4 K temperature range for a representative sample in the $K=0.2$ set with n very near n_c . Three fits to the data are shown, one of Eq. (1) restricted to data above 1.3 K, one of Eq. (1) restricted to data below 1.3 K, and a third fit using Eq. (2), also restricted to data below 1.3 K. Equation (2) gives a noticeably better fit over the full data range, even though only data with $T < 1.3$ K were used to construct the fit. We observe that the form of $\sigma(T)$ for the compensated samples with n near n_c appears to be

more complicated than for uncompensated Si:P.¹⁴ We obtained the values of $\sigma(0)$ listed in Table I by the following procedures. (1) For metallic samples sufficiently far above n_c , the fit of Eq. (1) to conductivity data between 1.3 K and 4.2 K yields accurate values of $\sigma(0)$. (2) For all metallic samples with fitted values of $\sigma(0) < 45 \Omega^{-1} \text{cm}^{-1}$ and a few other samples, additional data were taken in the range $50 \text{ mK} < T < 1.3 \text{ K}$. A fit of Eq. (1) to these low-temperature data yielded the improved values of $\sigma(0)$ recorded in Table I. (3) For samples very close to the transition, the function given as Eq. (2), with the exponent a as a fitting parameter, gives a more satisfactory fit to the data. We believe the values of $\sigma(0)$ derived from this procedure to be more accurate. These values are included in parentheses in Table I for the four samples of interest.

Even with the extension of the conductivity data to lower temperatures and use of the modified fitting function given as Eq. (2), the quality of the fits worsens as n approaches n_c and T approaches 0 K, making categorization of a sample as either metallic or insulating increasingly difficult. We therefore compute the logarithmic derivative $w(T) \equiv (d \ln \sigma) / (d \ln T)$. Zabrodskii¹⁵ and Möbius¹⁶ have previously noted the sensitivity of this function to the form of $\sigma(T)$. For example, for any metallic sample with $\sigma(0) > 0$, $w(T)$ will eventually tend toward zero as T approaches 0, whereas for an insulating sample with an exponential temperature dependence, $w(T)$ diverges as T approaches zero. Figure 1(b) displays values of $w(T)$ for sample $D-269$. We see that while the best fit of Fig. 1(a) gives a small nonzero value for $\sigma(0)$, the plot of $w(T)$ suggests that the true value of $\sigma(0)$ for sample $D-269$ is, in fact, zero.

Figure 2 shows a plot of $w(T)$ for six samples from crystal D , with $K=0.2$. The natural conclusion from this display is that the value of n_c for this sample set falls between the values $3.67 \times 10^{18} \text{ cm}^{-3}$ (sample $D-269$) and $3.72 \times 10^{18} \text{ cm}^{-3}$ (sample $D-280$). We remind ourselves, however, that small sample inhomogeneities may well compromise any attempt to locate the value of n_c with high precision.

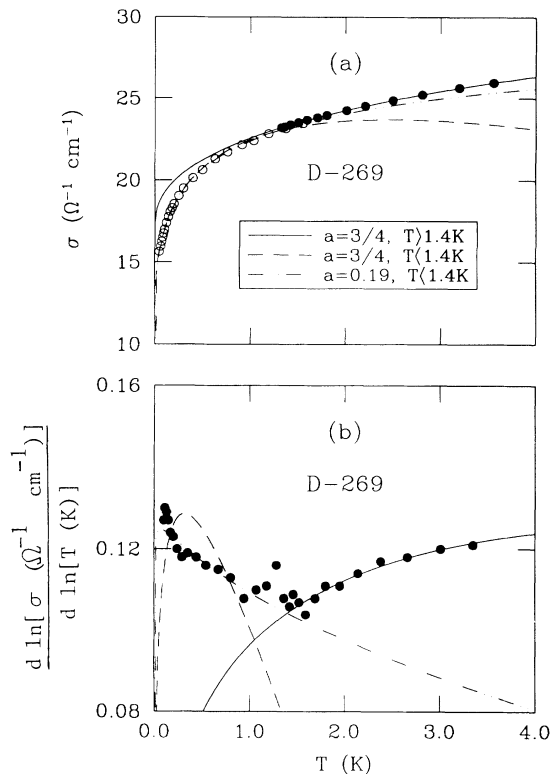


FIG. 1. Temperature dependence of (a) the electrical conductivity $\sigma(T)$ and (b) its logarithmic derivative $w(T) \equiv d \ln \sigma / d \ln T$, a dimensionless quantity for sample $D-269$. Also shown are various fits described in the text. The fitting curves in (b) are identical to those in (a), transformed to the logarithmic derivative scale.

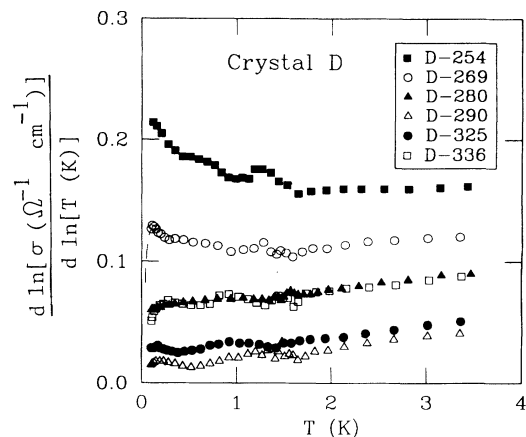


FIG. 2. Temperature dependence of $w(T) \equiv d \ln \sigma / d \ln T$ for six samples from crystal D . The dashed line for sample $D-269$ represents some data taken at the lowest available temperatures. The sharp decrease in $w(T)$ is likely due to sample heating.

B. Critical behavior of the zero-temperature conductivity

Figures 3 and 4 show values of $\sigma(0)$ plotted versus carrier concentration n for the three sample sets *A*, *B*, and *D*. Figure 4 reproduces data from HTH as well as the results of measurements in the 50 mK to 1.3 K range for several samples not included in HTH.

We note that the Czochralski growth process produces slowly changing values of K as one moves down a particular ingot. This change is a consequence of the differing segregation coefficients for phosphorus and boron. Thus, K slowly increases as one moves from right to left along the curves in Figs. 3 and 4. We label the particular value of K at $n = n_c$ as K_c .

Shown in Fig. 3 are two fits of the scaling theory expression, Eq. (3), to data for crystal *D*. One fit uses values of $\sigma(0)$ derived from the fitting function Eq. (1) and the other uses values of $\sigma(0)$ derived from Eq. (2). The substantial difference in the resulting values of the exponent μ , 0.9 and 0.5, emphasizes the sensitivity to procedures used to obtain values of $\sigma(0)$ for samples with n very near n_c . The fact that we had a number of samples from crystal *D* with rather closely spaced values of n very near n_c has highlighted this effect for these $K = 0.2$ samples.

Figure 4 shows data for the more highly compensated samples from crystals *A* and *B*. Fewer samples with n near n_c were available for these larger values of K , so that the rather exhaustive examination of $\sigma(T)$ carried out for the *D* samples was not appropriate. The scaling theory fits over this wide range of n give $\mu = 0.95 \pm 0.1$ for sample sets *A* and *B*.

As in HTH, the analysis scheme leading to Figs. 3 and 4 is based on the assumption that the single-parameter scaling theory² is valid. As long as the scaling parameter g , the length-dependent conductance, is a smooth func-

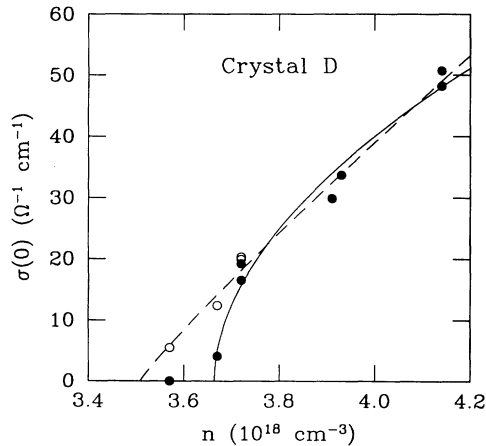


FIG. 3. Values of the zero-temperature electrical conductivity $\sigma(0)$ as a function of carrier concentration n for crystal *D*. The filled circles represent our best estimates for $\sigma(0)$, using Eq. (1) for the upper four samples and Eq. (2) for the lower four samples. The open circles are the results from fits of Eq. (1) for the lower four samples. The solid and dashed lines are scaling theory fits giving $\mu = 0.5$ and $\mu = 0.9$, respectively. [For the solid lines, the parameters in Eq. (3) are $\sigma_0 = 141 \Omega^{-1} \text{cm}^{-1}$, $n_c = 3.66 \times 10^{18} \text{cm}^{-3}$, $\mu = 0.53$; for the dashed line, $\sigma_0 = 234 \Omega^{-1} \text{cm}^{-1}$, $n_c = 3.51 \times 10^{18} \text{cm}^{-3}$, $\mu = 0.91$.]

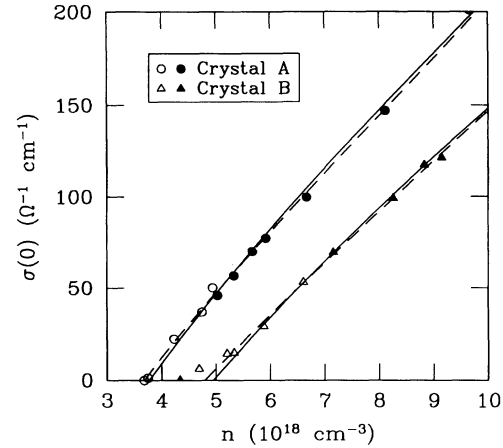


FIG. 4. Values of $\sigma(0)$ as a function of carrier concentration n for crystals *A* and *B*. Open symbols indicate that the value of $\sigma(0)$ was derived from data extending down to 50 mK. The dashed lines are fits of the scaling theory prediction, Eq. (3). [For crystal *A*, the fitting parameters in Eq. (3) are $\sigma_0 = 125 \Omega^{-1} \text{cm}^{-1}$, $n_c = 3.69 \times 10^{18} \text{cm}^{-3}$, $\mu = 0.93$; for crystal *B*, $\sigma_0 = 136 \Omega^{-1}$, $n_c = 4.80 \times 10^{18} \text{cm}^{-3}$, $\mu = 0.97$.] Solid lines are fits of Eq. (4), representing the Boltzmann conductivity modified by weak localization corrections. [For crystal *A*, the fit of Eq. (4) gives $l = 65.4 \text{ \AA}$, for crystal *B*, $l = 59.7 \text{ \AA}$.]

tion of n and K , either n or K or some combination of them can be varied to extract the conductivity exponent from a plot of $\sigma(0)$. If, in our compensated samples, both n and K are varying smoothly as the transition is approached, a plot of $\sigma(0)$ as a function of either n or K separately should yield the same exponent. A further discussion of this point is given in HTH and in Ref. 10.

Figure 4 also shows fits of Eq. (4), the standard weak localization prediction which includes perturbative corrections to the Boltzmann conductivity.⁶ For the fit, the value of the mean-free path l is taken to be independent of the value of n . This simplification seems qualitatively sensible, since effects of screening and of additional scattering centers work in opposite directions. An additional term for Eq. (4) proportional to $1/(k_F l)$ has been proposed.¹⁷ We find, however, that its inclusion does not significantly alter the quality of the fits. Although these fits have only one adjustable parameter, the mean-free path l , they describe the data for crystals *A* and *B* as well as the scaling theory fits of Eq. (3). The fact that our data can be described very well by Eq. (4) for most of our metallic samples of crystals *A* and *B* leads us to suggest that the critical region is limited to values of n such that $n/n_c < 1.1$. Since our data for crystal *D* cannot be fit well by Eq. (4), we presume that these samples lie mostly in the critical region.

Because of our interest in establishing the dependence of n_c upon the value of K , it was necessary to provide an unambiguous local link to uncompensated Si:P. Figure 5 displays values of $\sigma(0)$ versus n for Si:P, including both the literature data from Ref. 4 and our spot checks. The numerical scale for n for our data is based on our new $\rho(296 \text{ K})$ versus n scale.^{18,19} Values of n for the data from Ref. 4, which were derived using the older Mousty

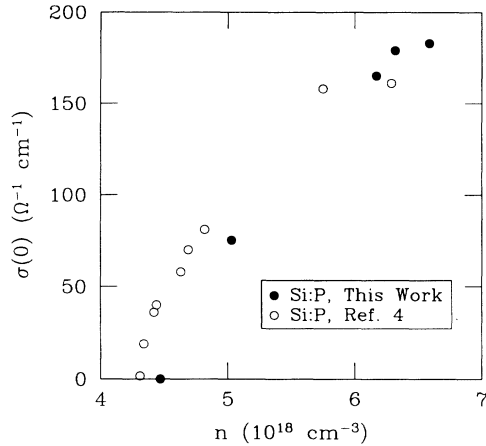


FIG. 5. Values of $\sigma(0)$ as a function of carrier concentration n for uncompensated Si:P, obtained from Ref. 4 (open circles) and recent measurements (solid circles). There is good agreement between the two data sets when a consistent concentration scale is used.

scale,²⁰ have been adjusted upward by 15% to conform to the new scale. A fit of Eq. (3) to our data gives a value $\mu = 0.6 \pm 0.1$, in good agreement with the value from Ref. 4.

The reassessment of the calibration scale used for determinations of values of n in uncompensated Si:P has led us to set the value of n_c at $4.5 \times 10^{18} \text{ cm}^{-3}$. We remark that this value mutes the discomfort occasioned by an earlier comparison of values of n_c in uncompensated Si:P and Si:As.²¹ With the new value of n_c for Si:P and the refined value of n_c for Si:As obtained by Shafarman, Koon, and Castner,²² the ratio $(n_c)_{\text{As}}/(n_c)_{\text{P}}$ is shifted to a value of 1.9 from the earlier²¹ value of 2.3. The new value is closer to the predicted value of 1.64 which is derived from an argument²¹ based on effective Bohr radii.

C. Dependence of n_c on K

Figure 6 displays the results of our investigations of the dependence of the critical concentration n_c on compensation ratio K . One naturally expects the increasing disorder in the compensated samples to demand higher electron concentrations to achieve a metallic state. Beyond that qualitative statement, no full theory for $n_c(K)$ exists, so far as we know. The early theoretical model developed by Shklovskii and Efros³ is appropriate for values of K near unity, but is not obviously applicable to the range of K which we have explored. In Sec. IV we speculate on a possible reason for the apparent small decrease in n_c for the D samples relative to $K = 0$.

Considerable information on the K dependence of n_c for several compensated Ge systems is available from the work of Zabrodskii.²³ In general, the dependence of n_c on K for the Ge systems is stronger than, but qualitatively similar to, the behavior for Si:(P,B). We note that for Ge:As, Zabrodskii's value of n_c at $K = 0.3$ was unchanged from that at $K = 0$, resembling the behavior of our data for Si:(P,B) displayed in Fig. 6.

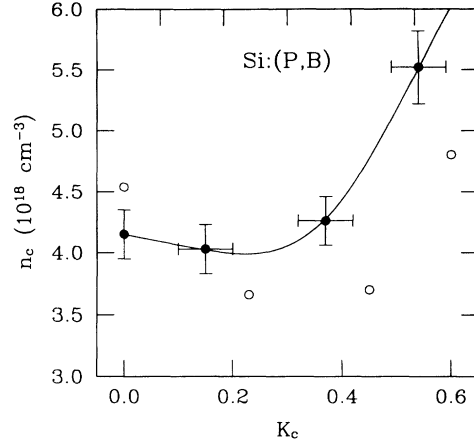


FIG. 6. Variation of the critical carrier concentration n_c with compensation ratio K . Open circles represent original values obtained as described in the text, while the solid circles are improved estimates (see Appendix). The solid line is only a guide to the eye.

Some commentary on methods for establishing the values of n_c given in Fig. 6 is appropriate. The anchor point at $K = 0$ (open circle) is taken from our measurements in uncompensated Si:P shown in Fig. 5. The numerical scale of n_c is established by our new ρ versus n scale^{18,19} for Si:P. For samples with $K > 0$, values of n_c are taken from the fits of Figs. 3 and 4 (open circles). The n scales for Figs. 3 and 4 were derived from room-temperature Hall measurements. The value of n is taken from the relationship $n = A(n)/R_H e$, where the functional form of the Hall scattering factor $A(n)$ is assumed to be unchanged from its well-studied^{19,24} behavior for uncompensated Si:P.

The solid points of Fig. 6 reflect the effects of adjustments made to achieve two purposes. (1) We need a consistent technique for establishing values of n_c for compensated and uncompensated samples. The solid point at $K = 0$ uses the value of n_c derived from measurements of the Hall coefficient $R_H(296 \text{ K})$ rather than the resistivity $\rho(296 \text{ K})$, thus mimicking the procedure for compensated samples. (2) It is desirable to include semiquantitative information we have garnered about changes in $A(n)$ values caused by compensation. The solid points for $K > 0$ result from adjusting the $A(n)$ curve to higher values on the basis of measurements of the infrared reflectivity and of the temperature dependence of R_H which are described in the Appendix. This adjustment in the $A(n)$ curve to generate adjusted values of n also affects K , since the value of K is determined by the relationship $K = N_B/N_P = 1 - n/N_P$.

Compensation in our samples has been achieved by means of adding both donors and acceptors in the Czochralski process. A parallel study of effects of compensation of Si:P via neutron bombardment has been carried out by Nishio and co-workers.²⁵ Much of their effort was directed towards the effects of compensation on properties on the insulating side of the $M-I$ transition. There is, however, some overlap on the metallic side of the $M-I$

transition. Their conclusions about the effects of compensation on the shape of the $\sigma(0)$ versus n curve match closely the results we display in Fig. 4. Concerning numerical values of n_c and their dependence on K , it is difficult to make direct comparisons between their results and ours because of differences in experimental methods for establishing values of n and K . Insofar as the dependence of n_c on K is concerned, a local relative scale would of course be satisfactory. However, they appear not to have accumulated sufficient data in metallic samples to generate a plot such as our Fig. 6.

IV. SUMMARY AND CONCLUSIONS

We now summarize new information derived from the study reported here concerning significant changes in details of the M - I transition in compensated samples in comparison with uncompensated Si:P.

(1) While the value of n_c does eventually rise sharply as K increases, in qualitative agreement with a theoretical model developed by Shklovskiĭ and Efros³ which is appropriate for values of K near unity, that rise appears to be preceded by a small dip or, at least, by a flat section in the n_c versus K_c plot of Fig. 6. We can only speculate about the reason for this interesting dip. It may be that the existence of the higher concentration of local moments in the compensated samples implied by the spin susceptibility measurements of Hirsch and Paalanen²⁶ suppresses the coherent backscattering associated with the weak localization model of transport in these systems. Once this contribution has been fully suppressed, the expected shift upwards in n_c occurs as disorder becomes even stronger.

(2) For compensated samples with n values near n_c , the temperature dependence of σ in the range $50 \text{ mK} < T < 4 \text{ K}$ departs significantly from the form $\sigma = \sigma(0) + mT^{1/2} + BT^{3/4}$. This relationship does give a good description of samples with $n/n_c > 1.1$.

(3) Use of the logarithmic derivative $(d \ln \sigma)/(d \ln T)$ to characterize the conducting properties is a sensitive test of the division between metallic and insulating samples. Use of this function with our measurements suggests that one tends to underestimate the value of n_c in the compensated samples if one uses the scaling form, Eq. (3), over a wide range of values of n/n_c .

(4) Fits to the data from the new set of samples with $K=0.2$ by the scaling theory expression, Eq. (3), give a value $\mu = 0.5 \pm 0.1$, using our best estimates of $\sigma(0)$. This value agrees with the value for uncompensated Si:P.²⁷ However, because of the questionable reliability of the extrapolation to $T=0 \text{ K}$, which is required to obtain the values of $\sigma(0)$ displayed in Fig. 3, we do not wish to place much weight on the apparent agreement.

(5) For the more heavily compensated samples, the weak localization expression given as Eq. (4) provides a fit to the experimental data for $\sigma(n, T=0)$, which is at least as satisfactory as the scaling theory expression Eq. (3). It is our opinion that the scaling theory is not applicable to most of the data shown in Fig. 4, but rather is only valid in a small range of n just above n_c .

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APPENDIX: DETERMINATION OF DOPANT AND CARRIER CONCENTRATIONS

There are many inconsistencies in values of n and n_c given in the literature for studies of the M - I transition in heavily doped Si and Ge. An important source of this inconsistency is the use of different schemes to derive dopant concentrations on the basis of measurements of the electrical transport properties, ρ and R_H . We urge workers in this field to regularly include actual experimental values of ρ and R_H at specified temperatures in order to provide unambiguous markers to which other workers may connect.

In this appendix, we give details about the determination of the carrier concentration n and compensation ratio K in our samples of Si:(P,B). We assume that all phosphorus and boron impurities are substitutional and electrically activated, i.e., the phosphorus concentration N_P and boron concentration N_B represent the concentration of shallow donors and acceptors, respectively. Since all of our samples are metallic or very nearly metallic, we also assume that all impurities are ionized at room temperature.²⁸ Thus, the carrier concentration n is equal to the excess donor concentration, i.e., $n = N_P - N_B$. Next, we consider the compensation ratio $K \equiv N_B/N_P$. For all of our samples, we have determined N_P by neutron activation analysis (NAA) to an accuracy of $\pm 5\%$ relative to standards with known phosphorus content. In our case, these standards consisted of several samples of uncompensated Si:P, whose room-temperature resistivity $\rho(296 \text{ K})$ was measured. The connection between resistivity and phosphorus concentration was made via a newly generated conversion scale^{18,19} based on a reexamination of a previous scale published by Thurber *et al.*²⁹ and other published data.²⁴ We have adjusted all values of N_P from HTH to reflect the upward revision of N_P of the NAA standard by 20%. The published values of n for the data of Rosenbaum *et al.*²⁷ on Si:P, which were determined using the older Mousty resistivity scale,²⁰ have also been adjusted to conform to the new scale. This upward adjustment of 15% is reflected in the data plotted in Fig. 5.

Unfortunately, we have not been able to make a direct determination of N_B which is sufficiently reliable and accurate for our purposes. Therefore, we chose to measure $R_H(296 \text{ K})$ in order to obtain the carrier concentration n .

We use the relation $R_H = A/ne$, where the Hall scattering factor A depends on the relative magnitudes of the relevant scattering mechanisms. Thus, A can be expected to be a function of n and K . The behavior of A as a function of n has been studied extensively for uncompensated Si:P ($K=0$).^{19,20,24} As a first approximation, we tried applying the known functional form of $A(n)$ for uncompensated Si:P to our compensated samples. In HTH, we used only data from Ref. 20, but we now use more accurate and complete data for $A(n)$ from several sources.^{19,24} However, it has become apparent to us that the values of A , and hence n , obtained in this way were underestimates. We note that it is theoretically plausible³⁰ that compensation leads to an increase in the value of A at a given n due to the increased dominance of ionized impurity scattering over lattice scattering.

We performed two experiments that support our assertion that the effect of compensation is to increase the

value of A . First, we measured¹² the temperature dependence of the Hall coefficient. As the temperature is decreased, lattice scattering decreases relative to ionized impurity scattering, so that A is expected to increase. We have found this increase in A to be smaller in the compensated samples, indicating that the value of A at room temperature was already larger than that for the uncompensated samples. Second, measurements of the infrared reflectance show that for samples with the same R_H (296 K), but different values of K , the plasma edge occurs at higher frequencies for samples with higher K . The higher value of n indicated by the increase in the plasma frequency at a given value of R_H (296 K) shows that A increases with increasing compensation. Both experiments mentioned above indicate that the effect of compensation is to increase the value of A at a given n by approximately 10% at $K=0.2$ and by 15% or more at $K \geq 0.4$.

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