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Critical behavior of the zero-temperature conductivity in compensated silicon, Si:(P,B)

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The zero-temperature electrical conductivity, $\sigma(0)$, of samples of Si:(P,B) has been obtained by extrapolation from measurements at temperatures of 100 mK and above. The compensation ratio K, defined as the ratio of acceptor to donor concentrations, ranges from 0.2 to 0.5. Naturally occurring gradients in the electron concentration n and values of K in melt-grown crystals provide sets of samples whose properties vary smoothly through the metal-insulator transition. Following a single-parameter scaling theory of localization, we analyze our data in terms of a relation $\sigma(0)=\sigma_0(n/n_c-1)^{\mu}$. Alternatively, we use the experimental variable $\sigma(296)$, the room-temperature conductivity, in place of the electron concentration n. Values of the conductivity exponent μ for three crystals range from 0.79 to 0.91, with estimated errors of ±0.08. No clear evidence for a dependence of μ on the compensation ratio K is found in the range of K covered by our samples.

Study of the behavior of the zero-temperature electrical conductivity, $\sigma(0)$, in disordered systems which undergo a metal-insulator (M-I) transition has been an active area of research. As the transition is approached from the metallic side, a scaling theory of localization[1] predicts that $\sigma(0)$ should drop to zero in a continuous manner according to the relation

$$\sigma(0)\propto[g(L_0)/g_c-1]^{\mu} . \quad (1)$$

In this expression, $g(L_0)$ is a conductance on a microscopic length scale L_0, g_c is the value of conductance for a sample exactly at the transition, and μ is the conductivity exponent. If the single scaling parameter g is a smooth function of the electron concentration n and the degree of compensation, then a linear expansion of g about g_c allows one to use the experimentally accessible variable n as the scaling variable, such that

$$\sigma(0)=\sigma_0(n/n_c-1)^{\mu} . \quad (2)$$

Searches for the value of μ for various systems using Eq. (2) have been extensive.[2] A summary of the results is that almost all disordered M-I transition systems exhibit values of μ less than but near unity, with the exception of singly doped Si:P ($\mu=0.48\pm0.07$)[3], Si:As (0.61 ± 0.05),[4,5] Ge:Sb (0.7 ± 0.2)[6], and the double donor system Si:(As,P) (0.7 ± 0.2).[7] See Table I for a summary of exponents found for various systems.

This paper reports experimental conductivity results for the compensated material Si:(P,B). Comparison of our results with those of Si:P provides a direct test of the effects of compensation on the electrical properties near the M-I transition. We find the conductivity exponent for Si:(P,B) to be $\mu\approx0.8-0.9$ for moderate compensation, which clearly differs from the value of $\mu=0.5$ for uncompensated Si:P. However, for our samples, we do not find a significant dependence of μ on the degree of compensation or our choice of scaling variable.

Compensation allows one to vary the amount of disor-

TABLE I. Values of the conductivity exponent μ for a variety of systems and various compensation ratios K. Wherever a range of K is listed, the upper limit is the critical value K_c, the compensation ratio at the M-I transition. The numbers in parentheses listed for each Si:(P,B) crystal are the values of μ obtained by using $\sigma(296)$ as the scaling variable instead of n.

System	μ	K	Reference
Si:P	0.48 ± 0.07	0	3
Si:As	0.61 ± 0.05	0	4,5
Si:(As,P)	0.7 ± 0.2	0	7
Si:(P,B)	$0.87\pm0.08(0.79)$	0.24–0.43	This work, crystal A
Si:(P,B)	$0.90\pm0.08(0.91)$	0.34–0.52	This work, crystal B
Si:P	≈1	variable	20
Ge:Sb	0.7 ± 0.2	≤0.05	6
Ge:Sb	≈1	≈0.2	6
Ge:Sb	≈1	≈0.35	6
Ge:(Ga,As)	0.8 ± 0.15	0 to 0.35	16
Ge:(Sb,In)	0.9 ± 0.1	≈0.3	17
Ge:Sb	0.9 ± 0.1	≈0.2	19

der in a system. An n-type semiconductor with donor concentration N_D and acceptor concentration N_A will have a carrier concentration $n = N_D - N_A$. One parameter which measures the degree of compensation is the compensation ratio $K = N_A / N_D$. A compensated system may be envisioned as a sea of electrons of density n among positively and negatively charged scattering centers with total density $N_D + N_A = n[(1+K)/(1-K)]$. Thus, compensation may be used to increase the ionized scattering center density at a particular value of n, relative to a singly doped system with $K=0$. The possible dominance of qualitatively different scattering mechanisms due to the enhanced disorder and increased number of scattering sites seem likely sources[8] for the change in μ from its $K=0$ value.

EXPERIMENTAL DETAILS

Our samples were cut from Czochralski-grown crystals of n-type Si:(P,B).[9] This growth process results in a crystal in which n increases and K decreases smoothly along its length. Fluctuations in concentration of one or both dopants produce some scatter in values of n and K about the local average values. Resistivity mappings on 380-μm-thick wafers were done with a standard four-point probe technique in order to locate regions of sufficient homogeneity. Clover-leaf shaped samples were cut ultrasonically from these regions. These samples were 8 mm in diameter, with a central intact circular region of 4 mm diameter. The spread in room-temperature resistivity values, $\rho(296)$, over a typical sample was 5%, while the central region, which primarily controls the values of ρ measured by the van der Pauw technique, typically had a 2% spread in $\rho(296)$. This spread in ρ corresponds to a 1.5% variation in n values.

The phosphorus concentration was measured by thermal neutron activation of a sample together with a standard of known concentration. The standards were wafers of Si:P whose phosphorus concentration was determined by using the calibration curve relating $\rho(296)$ and N_D developed by Thurber *et al.*[10] The carrier concentration for our samples was determined by measuring the room-temperature Hall coefficient R_H and using the relation $n = A(n)/R_H e$. The value of the Hall scattering factor A was determined self-consistently using the A-versus-n curve for Si:P published by Mousty *et al.*[11] The typical value of A used was 1.15. $A(n)$ is a slowly varying function of n for Si:P. It seems likely that $A(n)$ will also vary slowly at a given n as a function of K. We estimate the random error in our values of n to be ±2%.

Values of σ from 1.3 K to room temperature were measured using the system described previously.[12] Certain samples, particularly those near the transition, were measured to temperatures below 200 mK using a Linear Research model LR-400 resistance bridge. Figure 1 shows typical data for some representative samples.

The naturally occurring gradients in n and K along a compensated crystal provide a set of samples whose properties vary smoothly through the M-I transition. We obtained two suitable crystals, designated A and B, each of which yielded a set of samples just on the metallic side of the transition. Measured properties of these samples are listed in Table II. Also listed is complementary data on a third crystal, named C, to be discussed below. The sample numbers correspond to the number of the wafer from which they were cut, counted from the seed end of the crystal.

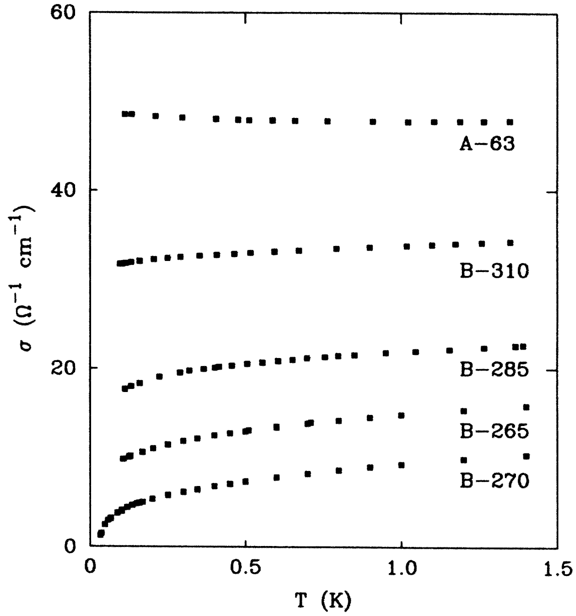

FIG. 1. Electrical conductivity σ as a function of temperature T for representative samples of Si:(P,B). Sample characteristics are given in Table II.

To obtain values of $\sigma(0)$, we used an extrapolation procedure similar to that used previously by Thomas *et al.*[13] The best fit to our data below 4.3 K was obtained using the form

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

Theoretically, the $T^{1/2}$ term results from the effect of electron-electron (e-e) interactions on the density of states near the Fermi level in a disordered metal. The term involving $T^{3/4}$ is a weak localization correction due to inelastic e-e collisions. This term arises from an e-e inelastic scattering rate proportional to $T^{3/2}$, as was proposed for disordered systems by Schmid.[14] While the theories of disorder-enhanced e-e interactions and weak localization have been derived for the weak scattering limit and would not be expected to be valid at the M-I transition, we note that similar fitting functions have been successfully employed previously near n_c.[3-7,13] A fuller discussion of the fitting procedure as well as values of m and B can be found elsewhere.[12,15]

Extrapolations to $T=0$ K from $T \approx 1.4$ K for samples close to the transition tend to overestimate values of $\sigma(0)$.[4] All samples from crystals A and B with values of $\sigma(0)$ below 45 $\Omega^{-1}\,\text{cm}^{-1}$ were measured to temperatures below 200 mK. At values of 45 $\Omega^{-1}\,\text{cm}^{-1}$ and greater,

TABLE II. Characteristics of Si:(P,B) samples. Values of n, K, and $\sigma(0)$ are obtained as described in the text; $\sigma(296)$ is measured directly.

Sample	n (10^{18} cm^{-3})	K	$\sigma(296)$ (Ω^{-1}cm^{-1})	$\sigma(0)$ (Ω^{-1}cm^{-1})
A-1	3.39	0.43	37.4	0.0
A-9	3.45	0.4	40.2	1.3
A-87	4.34	0.39	47.4	37.8
A-63	4.51	0.35	50.6	50.1
A-64	4.59	0.31	49.7	45.9
A-73	4.87	0.34	52.7	56.7
A-77	5.16	0.31	56.4	69.9
A-111	5.40	0.29	58.8	77.2
A-105	6.08	0.24	65.5	99.7
A-130	7.40	0.19	81.2	147
A-194	8.88	0.23	99.0	201
B-270	3.96	$\approx$0.55	29.7	0.0
B-265	4.26	$\approx$0.55	33.3	6.1
B-285	4.87	0.52	36.3	15.4
B-310	5.33	0.50	41.6	31.3
B-312	6.03	0.47	47.9	53.1
B-322	6.54	0.41	53.2	69.3
B-348	7.57	0.34	63.1	99.0
B-320	8.05	0.31	69.4	117
B-354	8.39	0.37	71.0	121
C-89	4.14	0.53	34.6	0.0
C-92	4.29	0.52	36.6	9.2
C-94	4.65	0.53	39.2	17.5
C-138	4.77	0.51	39.1	22.3
C-112	4.84	0.53	41.1	26.0
C-115	5.23	0.51	44.7	38.5
C-133	5.47	0.47	44.5	40.5
C-135	5.67	0.45	46.9	47.3
C-136	5.70	0.45	48.2	51.8

values of $\sigma(0)$ obtained by extrapolation from 200 mK or 1.4 K agreed to within 4%. For samples with $\sigma(0) < 10$ Ω^{-1}cm^{-1}, the extrapolation using Eq. (3) becomes questionable. We find no clear distinction between the functional form of $\sigma(T)$ for sample B-265 and that for the insulating sample B-270. It is possible that the true value of $\sigma(0)$ for sample B-265 is, in fact, zero.

DATA ANALYSIS AND DISCUSSION

To make progress in the analysis of our data, we assume that the critical behavior of $\sigma(0)$ is controlled by the single parameter $g(L_0)$ as in Eq. (1). Experimentally, we obtain values of $\sigma(0)$ for samples characterized by n and K. However, we have no knowledge of $g(L_0)$ for our samples, so that we cannot extract the value of μ from Eq. (1). We therefore proceed to assume that g is a smooth function of n and K. This enables us to use n as the control variable by making a linear expansion of g about g_c, such that

$$g - g_c = \left.\frac{dg}{dn}\right|_{n_c} (n - n_c) \; . \qquad (4)$$

The value of dg/dn depends on the functional relationship between K and n. Substituting Eq. (4) into Eq. (1), we obtain Eq. (2) with $\sigma_0 \propto dg/dn\,|_{n_c}$. Note that the value of the conductivity exponent μ is unaffected by the transformation from g to n. In particular, we can find the value of μ by fitting Eq. (2) to data from any set of samples with n near n_c and with smoothly varying values of K. Of course, the fitting parameters σ_0 and n_c will depend on how K changes with n in each data set.

The validity of the single-parameter scaling description of our values of $\sigma(0)$ can be tested by evaluating the conductivity exponent for different crystals. A plot of the extrapolated value of $\sigma(0)$ versus n is shown in Fig. 2. The samples are grouped according to the crystal from which they were cut. A fit of Eq. (2) is made to the data points for each crystal. The values of the fitting parameters σ_0, n_c, and μ are given in Fig. 2, along with the fits drawn through the data points.

Alternatively, we use the room-temperature conductivity $\sigma(296)$ as our scaling variable on the grounds that no special theoretical significance is attached to n. The scaling relation becomes

$$\sigma(0) = \sigma_0[\sigma(296)/\sigma_c - 1]^{\mu} \; . \qquad (5)$$

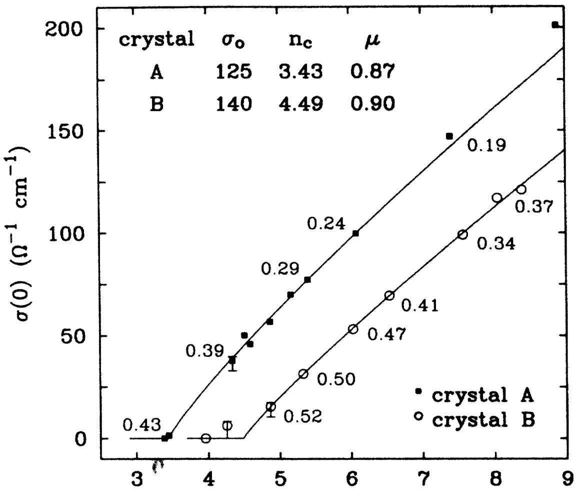

FIG. 2. Values of $\sigma(0)$ for crystals A and B as a function of carrier concentration n. The solid lines are fits of Eq. (2) to all data for which $n < 2n_c$ except sample B-265 ($n = 4.26\times10^{18}$ cm^{-3}), whose value of $\sigma(0)$ may be zero (see text). The values of the fitting parameters σ_0, n_c, and μ are given in the inset table. Units for σ_0 and n_c are $\Omega^{-1}\,\text{cm}^{-1}$ and 10^{18} cm^{-3}, respectively. The numbers next to selected data points are values of the compensation ratio K for those samples.

The value of μ in Eq. (5) should be the same as before, while the values of the fitting parameters σ_0 and σ_c depend on the details of the transformation between g and $\sigma(296)$. A plot of $\sigma(0)$ versus $\sigma(296)$ along with the results of fits of Eq. (5) to the data are shown in Fig. 3. Results for crystal C are included, but are more uncertain because the measurements on which the results are based were less complete than those for crystals A and B.

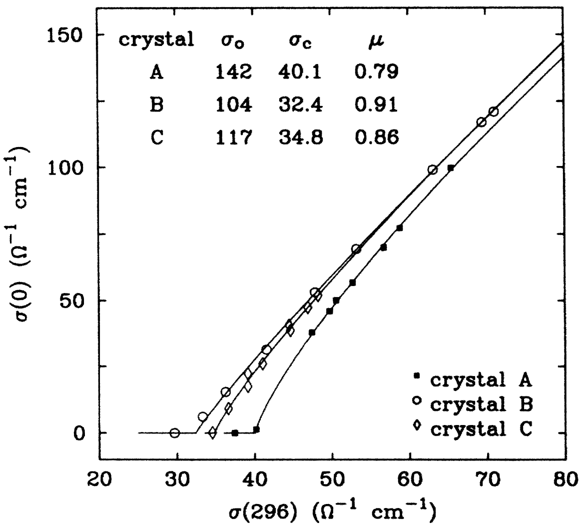

FIG. 3. Values of $\sigma(0)$ for crystals A, B, and C as a function of room-temperature conductivity $\sigma(296)$. Solid lines are fits of Eq. (5) to all data shown except that for sample B-265. Note that the two data points of Fig. 2 with $n > 2n_c$ are not shown here. The values of the fitting parameters σ_0, σ_c, and μ are given in the inset table. Units for σ_0 and σ_c are $\Omega^{-1}\,\text{cm}^{-1}$.

We have empirically found Eqs. (2) and (5) to fit our data up to values of $n \approx 2n_c$. We note that it is difficult to determine, *a priori*, the size of the region over which Eq. (2) or Eq. (5) is valid. Our values of μ for crystal A are derived from data covering the range $1.0 < n/n_c < 1.77$, and for crystal B the range $1.08 < n/n_c < 1.87$. We find values of μ ranging from 0.79 to 0.91 for our sets of samples, using both n and $\sigma(296)$ as scaling variables. The uncertainty in μ for each fit is ±0.08. Thus, for values of K between 0.2 and 0.5, our data is consistent with a constant value of the exponent μ and hence with a single-parameter scaling theory. A continuous change in the value of μ from 0.5 to 1.0 has been suggested by Thomas *et al.*,[6] on the basis of data for compensated Ge. Although our values of μ hint at a small dependence on K, the estimated uncertainty is sufficiently large that no firm conclusion can be drawn concerning such a K dependence. Our data does not, of course, rule out a continuous change in μ occurring between $K = 0$ and $K \approx 0.2$. If μ does indeed vary continuously with K, then a single-parameter scaling theory is not valid.

Our results are consistent with those drawn from several studies of other compensated semiconductors. Zabrodskiĭ and Zinov'eva[16] obtained a value of $\mu = 0.8\pm0.15$ for Ge samples which covered a range in K from 0 to 0.35. Allen, Wallis, and Adkins[17] obtained low-temperature conductivity data for Czochralski-grown crystals of Ge:(Sb,In) with $K \approx 0.3$. We have analyzed their data[18] using the same technique as described here and obtain $\mu \approx 1$ for samples in the range $1.14 < n/n_c < 2.16$. Field and Rosenbaum[19] quoted a value of $\mu = 0.9\pm0.1$ for lightly compensated samples of Ge:Sb with an estimated compensation ratio of $K \approx 0.2$. In a recent study, Sasaki, Nishio, and Kajita[20] reported a value $\mu \approx 1$ for Si:P which had been compensated by neutron damage. The exponents quoted above are summarized in Table I.

Examining the values of n_c given in Fig. 2, one notes a substantial difference between crystals A and B. Moreover, the value for crystal A, $n_c = 3.4\times10^{18}$ cm^{-3}, is 10% smaller than the value for uncompensated Si:P, $n_c = 3.75\times10^{18}$ cm^{-3}. This observation is counterintuitive, and we offer two possible explanations. First, there may be a weak link in our method of determining n, namely, the assumption that the Hall scattering factor is the same for Si:(P,B) as for Si:P. We note, however, that the validity of our exponent determination is independent of the correctness of this assumption. Second, there could be a parameter other than n and K which also influences the value of $\sigma(0)$. For example, this extra parameter might be spatial correlations between donor and acceptor impurities. If the impurities tend to form donor-acceptor pairs, which have no net charge, the fluctuations of localized charge in a given region will be less than if the impurities were spatially uncorrelated. Such a reduction in the disorder would be expected to affect the value of $\sigma(0)$. In this context, we note in Fig. 3 an unexplained difference in the behavior of $\sigma(0)$ for crystals B and C, whose values of K are very similar.

In summary, the zero-temperature conductivity in compensated Si:(P,B) is well described by the scaling forms $\sigma(0)\propto(n/n_c-1)^{\mu}$ and $\sigma(0)\propto[\sigma(296)/\sigma_c-1]^{\mu}$ for $n<2n_c$. Our data as well as the determinations of μ from the data given in Refs. 16, 17, and 18 are consistent with the proposition that μ is independent of the value of K in the range $0.2<K<0.5$. We find $\mu\approx0.8$ to 0.9 in contrast to the $K=0$ value of $\mu=0.5$. An experimental determination of the behavior of μ in the range $0<K<0.2$ should provide more insight into the correct description of the transition.

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