Electrical conductivity of metallic Si:B near the metal-insulator transition

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(Received 9 September 1991)

The conductivity has been measured between 55 mK and 4.2 K in zero field and in magnetic fields up to 7.5 T of a series of uncompensated p-type Si:B samples with dopant concentrations near the critical concentration for the metal-insulator transition. Acceptor wave functions, which are derived in silicon from the degenerate light- and heavy-hole $J=\frac{3}{2}$ valence-band maxima at $k=0$ and a spin-orbit-split $J=\frac{1}{2}$ band, are quite different from donor wave functions associated with the six degenerate conduction-band minima at different equivalent points in the Brillouin zone. Despite this, the conductivity of Si:B is found to be quite similar in many ways to that of Si:P. The critical conductivity exponent for Si:B is close to $\frac{1}{2}$ as in Si:P and Si:As, rather than having the expected value of 1. The correction to the zero-temperature conductivity arising from electron-electron interactions is comparable in size, and the temperature dependence of the conductivity in various fixed magnetic fields is also found to be quite similar. For the range of dopant concentrations and experimental parameters of these investigations, the only important experimental difference between the two materials is the sign and size of the magnetoresistance. In contrast with Si:P, which has both positive and negative components, the magnetoresistance of Si:B is positive for all temperatures and magnetic fields studied. We attribute this to the strong spin-orbit scattering in p-type silicon associated with the degenerate valence bands.

I. INTRODUCTION

The transition from insulating to metallic behavior which occurs in doped semiconductors with increasing dopant concentration has been an interesting and active area of investigation for many years.[1] Studies of the conductivity have been particularly important for developing an understanding of the nature of the transition, and of the roles of localization and electron-electron interactions as the transition is approached. The critical behavior of the zero-temperature conductivity, the temperature dependence of the conductivity, as well as the magnetotransport and the Hall effect, have been studied in many different systems, including Si:P,[2,3] Si:As,[4,5] Si:Sb,[6] Ge:Sb,[7-9] and Ge:As.[10]

These investigations have centered largely on n-type materials, which are assumed to be typical and representative of all doped semiconductors. There are, however, interesting and important differences for p-type semiconductors which merit separate and careful attention. While n-type Si and Ge have, respectively, six and four degenerate conduction-band minima at different equivalent points in the Brilouin zone, their p-type counterparts have light- and heavy-hole $J=\frac{3}{2}$ valence-band maxima which are degenerate at $k=0$ and a third $J=\frac{1}{2}$ band shifted downward in energy by spin-orbit coupling. These differences have a number of interesting consequences. For example, the degeneracy and anisotropy of the conduction-band minima as well as intervalley scattering have been invoked[11] to account for some of the observed properties of Si:P and Ge:Sb near the transition. The valence bands, on the other hand, are essentially isotropic, and instead of intervalley scattering one must consider the effect of strong intervalence band scattering involving the heavy- and light-hole bands. Another important difference is that spin-orbit (S.O.) scattering is associated in n-type material with the dopant and is thus important only in the case of heavy impurities. In p-type material, spin-orbit effects derive instead from the nature of the host valence bands themselves. Scattering by impurities causes transitions among states with different J_z values between the degenerate heavy- and light-hole bands at a rate comparable with ordinary potential scattering,[12,13] so that spin-orbit scattering is always important, independently of the mass of the dopant. The importance of spin-orbit effects is manifested in a g value[14,15] in Si:B of 1.2 compared with a g factor in Si:P very close to the free-electron value of 2.

A detailed investigation of the transport behavior of p-type material, and a comparison with its n-type counterpart can thus yield interesting information concerning the role of spin-orbit scattering, anisotropy, and other factors associated with the nature of the bands. We have undertaken a systematic study of the transport properties of p-type Si:B containing boron concentrations near the critical concentration for the metal-insulator transition. In this paper, we present results of an investigation of the temperature-dependence of the conductivity in zero field and in magnetic fields up to 7.5 T. In addition, we summarize and expand on earlier results for the critical behavior of the zero-temperature conductivity.[16,17]

II. SAMPLES AND MEASUREMENTS

Wafers of approximate thickness 0.3 mm cut from Czochralski-grown crystals of Si:B were purchased from the Pensilco Corporation. The segregation coefficient,[18] defined as the ratio of the equilibrium concentration of

dopant in the crystal to that in the melt, is on the order of 0.8 for boron compared with 0.35 for phosphorus in silicon; comparable growth conditions should therefore yield considerably more homogeneous crystals of Si:B. Measurements on a 4-mm scale at different positions of a given 2-in.-diam wafer indicated random local fluctuations in boron concentration on the order of 1–2 %.

The room-temperature resistivity of a series of square-shaped (8×8 mm^2) samples measured in the van der Pauw[19] geometry is plotted as a function of the measured resistivity ratio ρ (4.2 K)/ρ(300 K) in Fig. 1(a). The Thurber[20] calibration was then used to establish a calibration curve for the resistance ratio versus boron concentration, as shown in Fig. 1(b). The resistivity ratio is a more sensitive function of the concentration than is the room-temperature resistivity, and is independent of sample geometry. An additional advantage is that it provides an accurate determination of relative concentrations, a matter of considerable importance for samples very near the transition. Not including the errors associated with the calibration provided by Thurber *et al.*,[20] we estimate there is a 1% uncertainty in the determination of the boron concentration of the samples used in these investigations.

Detailed field and temperature-dependent data were obtained for the samples listed in Table I. Bar-shaped samples were used of approximate dimensions $8\times1.5\times0.3$ mm^3, for which the boron concentrations were determined from measurement of the resistance ratio and use of Fig. 1(b). Electrical contacts which gave Ohmic behavior and low power dissipation required boron ion-implanted regions under the contact points, particularly for measurements below 1 K. Thin gold wires were attached to these heavily doped areas using an arc-discharge technique[21] commonly used for n-type silicon contacts. It was found that thermal anchoring by the standard method of attaching samples to a holder with grease or GE varnish caused stresses in the Si:B samples which produced substantial and uncontrolled changes in their properties. Thermal contact was therefore established by direct immersion in the helium fluid.

Measurements by standard four-terminal techniques were taken above 1.5 K in a standard ^{4}He glass Dewar equipped with a home-built 4 T superconducting magnet. Depending on the temperature range, the temperature was controlled by regulating the pressure above the liquid helium, or with a heater and BTI Model 1000 Conductance Bridge/Controller. Measurements between 55 mK and 1.5 K were made in a Oxford Model 75 dilution refri-

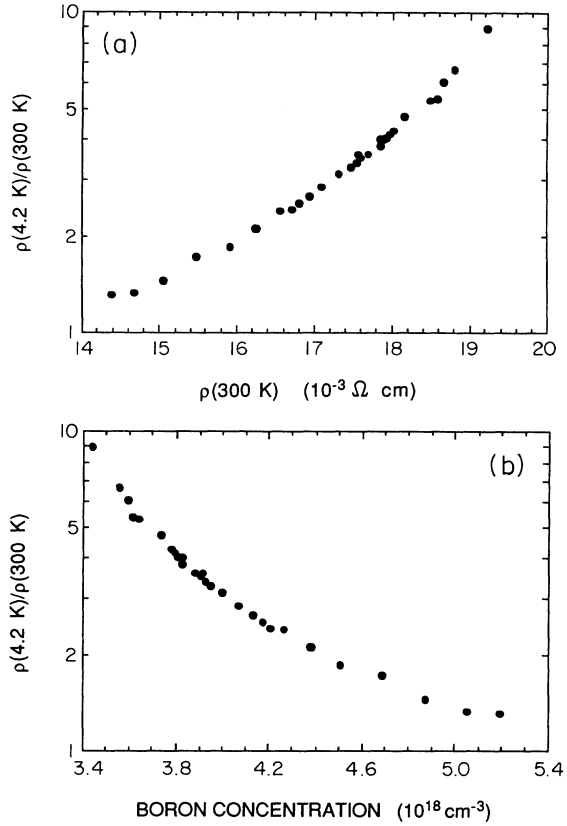

FIG. 1. (a) The ratio of the resistivities at 4.2 and 300 K, ρ(4.2 K)/ρ(300 K), as a function of ρ(300 K) plotted on a semilogarithmic scale. (b) The resistivity ratio, ρ(4.2 K)/ρ(300), vs boron concentration plotted on a semilogarithmic scale.

TABLE I. For the ten Si:B samples used in these studies, the table lists the room-temperature resistivity, ρ(300), the resistivity ratio, ρ(4.2 K)/ρ(300 K), the dopant concentration deduced from the calibration of Ref. 20, and from fitting the data to Eq. (1a), the coefficient m and the zero-temperature conductivity, $\sigma(0)$.

n (10^{18} cm^{-3})	ρ(300 K) (Ω cm)	ρ(4.2 K)/ρ(300 K)	m (Ω cm K$^{1/2}$)$^{-1}$	$\sigma(0)$ (Ω cm)$^{-1}$
4.11	0.017	2.684	9.49	9.5
4.20	0.0167	2.463	8.26	16.3
4.30	0.0165	2.270	2.05	22.9
4.38	0.0162	2.112	−0.14	26.8
4.57	0.0158	1.811	−4.79	39.3
4.72	0.0154	1.620	−7.78	48.5
4.86	0.0151	1.489	−6.95	52.9
4.95	0.0149	1.418	−7.43	57.1
5.01	0.0148	1.384	−7.07	59.2
5.22	0.0143	1.274	−7.15	64.7

gerator equipped with a 9-T magnet. The samples were immersed directly in the ^{3}He-^{4}He mixture in a glass-mixing chamber which extended to the center of the superconducting magnet. Over most of this range of temperature, data were obtained with a AVS-46 ac bridge of excitation frequency 15 Hz and minimum input voltage 10^{-5} V corresponding to an input power of 5×10^{-11} W for a 2-Ω sample. Measurements at the lowest temperatures required smaller power levels and were made with a PAR 124A lock-in amplifier using an excitation frequency 17.5 Hz, and a Model 118 preamplifier. Stable signals were obtained for inputs as low as 0.1 μV or approximately 10^{-14} W.

III. RESULTS AND DISCUSSION

A. Temperature dependence of the conductivity

The conductivities of the ten metallic Si:B samples listed in Table I are plotted in Fig. 2 as a function of temperature between 55 mK and 4.2 K. For samples with dopant concentrations well above the critical concentration n_c, the conductivity increases with decreasing temperature as is typical for a good metal. For concentrations near the metal-insulator transition, however, the conductivity decreases instead as the temperature is lowered. A similar change in the sign of $d\sigma/dT$ has been found in other doped semiconductors, including Si:P,[2] Si:As,[4] Si:P,B[22], and Ge:Sb,[7] and is thought to be associated with a breakdown of the Thomas-Fermi screening as the critical concentration is approached.[2]

The temperature variation of the conductivity is given by[1]

$$\sigma=\sigma(0)+\Delta\sigma_I+\Delta\sigma_L=\sigma(0)+mT^{1/2}+BT^{p/2}\ , \quad (1)$$

where the second term arises from electron-electron interactions[23,24] and the last term is the correction to the zero-temperature conductivity due to localization effects.[25,26] The temperature dependence of the latter is determined by the temperature dependence of the scattering rate $\tau_\phi^{-1}\approx T^p$ of the dominant dephasing mechanism. For electron-phonon scattering p is expected to be equal to 3, while in the case of inelastic electron-electron collisions, $p=2$ and $\frac{3}{2}$ for the clean and dirty[27] limit, respectively. The dephasing rate calculated by Belitz and Wysokinski[28] very near the transition gives $p=1$.

Fitting the data of Fig. 2 to Eq. (1) with all four parameters $\sigma(0)$, B, p, and m, allowed to vary freely yielded values of p between 1.3 and 1.65. Making the reasonable assumption that our materials are indeed representative of disordered metals, the fitting procedure was repeated

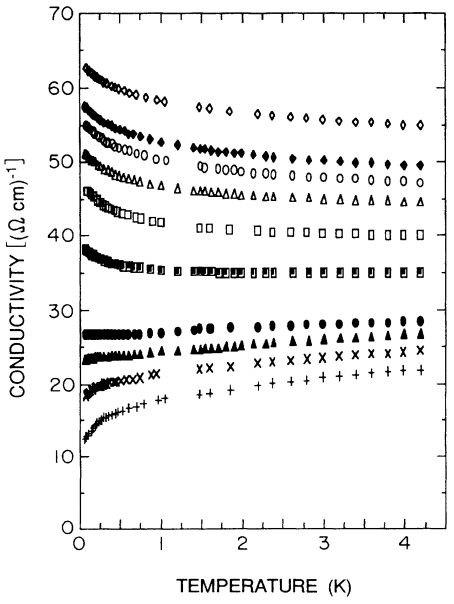

FIG. 2. Conductivity as a function of temperature of ten Si:B samples. In units of 10^{18} cm^{-3}, their boron concentrations are as follows: +, 4.11; ×, 4.20; ▲, 4.30; ●, 4.38; ■, 4.57; □, 4.72; △, 4.86; ○, 4.95; ♦, 5.01; ◇, 5.22.

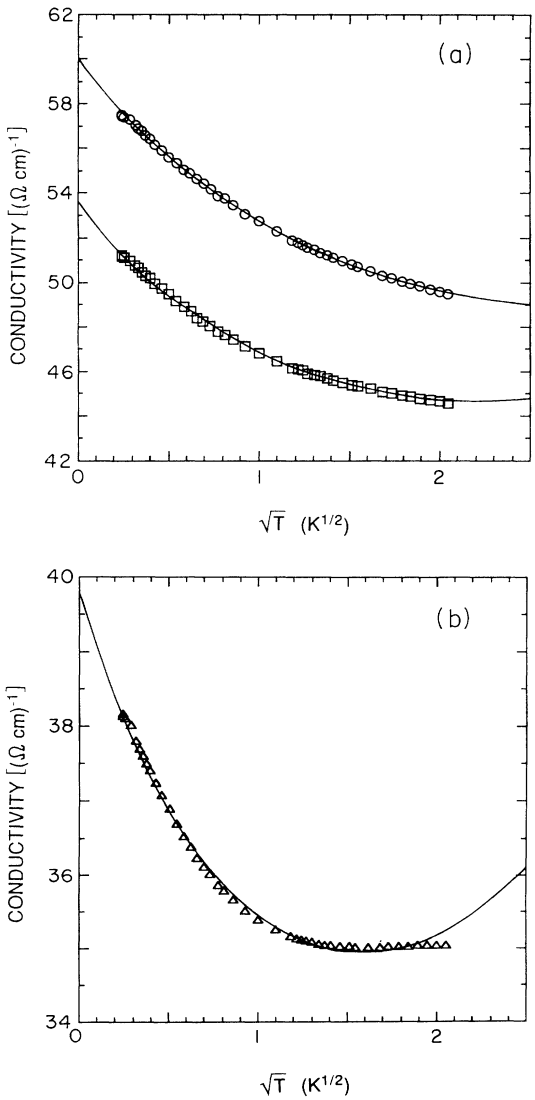

FIG. 3. Conductivity vs $T^{1/2}$. The solid lines are fits to Eq. (1). In units of 10^{18} cm^{-3}, the dopant concentrations are as follows: ○ 5.01; □, 4.86; △, 4.57.

with p fixed at the appropriate[27] value 1.5. As shown in Fig. 3, reasonable results are obtained for samples whose conductivities have negative slopes, $d\sigma/dT$, at low temperatures, that is, for boron concentrations greater than about 4.4×10^{18} cm^{-3}. One should note, however, that the values obtained for m and B depend on the breadth of the temperature interval used, indicating that a fit to three terms is not sufficient to describe the data very well over an extended range of temperature. Equation (1) provides better fits for samples at the higher concentrations far from the transition, and systematic deviations become apparent as the concentration is reduced. For samples with positive $d\sigma/dT$, deviations become quite large and negative values are obtained for B. Negative B's were also found for Si:As (Ref. 4) and Si:P,B (Refs. 22 and 29) for samples near the transition where the slope $d\sigma/dT$ of the conductivity at low temperature was positive. The parameter B obtained from fits to Eq. (1) is shown plotted as a function of boron concentration in Fig. 4 and is quite similar to that found with $p=2$ by Thomas *et al.*[7] in Ge:Sb and by Hirsch and Holcomb[22] using $p=\frac{3}{2}$ for Si:P,B.

A determination of the critical behavior of the zero-temperature conductivity, an issue of importance which will be discussed in more detail later, requires a reliable extrapolation of the conductivity to its zero-temperature limit, $\sigma(0)$. As pointed out earlier, Eq. (1) gives fits which are least reliable very near the transition, particularly if one includes an extended range of temperature. At the lowest temperatures, however, the term due to localization becomes relatively less important and the behavior is largely determined by the square-root behavior associated with electron-electron interactions. This is illustrated in Fig. 5, which shows the conductivity plotted as a function of $T^{1/2}$ for temperatures below 0.5 K. Omitting the localization term, the temperature range over which acceptable fits can be obtained to the two-term expression,

$$\sigma(T)=\sigma(0)+mT^{1/2} \tag{1a}$$

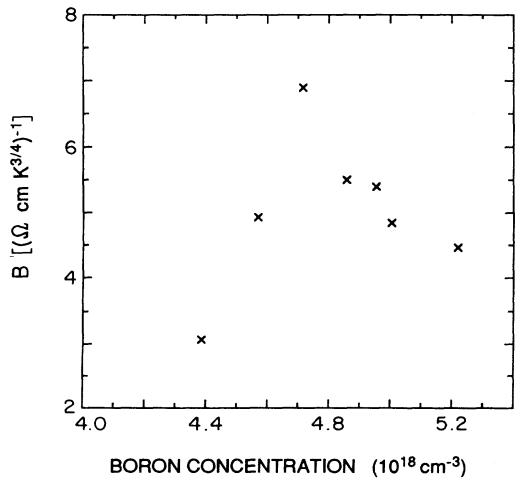

FIG. 4. The coefficient B of Eq. (1) plotted as a function of boron concentration.

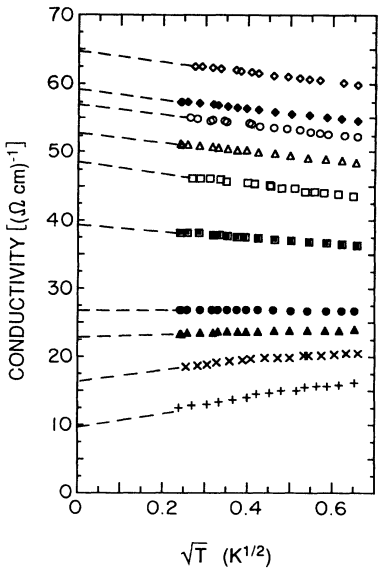

FIG. 5. The conductivity of ten metallic Si:B samples plotted as a function of $T^{1/2}$ for temperatures below 0.5 K. In units of 10^{18} cm^{-3}, the concentrations are as follows +, 4.11; ×, 4.20; ▲, 4.30; ●, 4.38; ■, 4.57; □, 4.72; △, 486; ○, 4.95; ♦, 5.01; ◇, 5.22. The dashed lines represent fits to Eq. (1a).

depends on how close a given sample is to the transition. Reliable fits could be made for most of the samples to about 500 mK. For the two samples very near the transition, however, it was necessary to limit the temperature range to below 200 mK. This allows a "fit" over a very restricted range of temperature, and thus provides neither a good test of the validity of the assumed $T^{1/2}$ behavior, nor a very reliable determination of $\sigma(0)$. A study of the detailed behavior of the conductivity and of $\sigma(0)$ very near the transition requires measurements to much lower temperatures. It is important to note, however, that the conclusions described later in this paper and published elsewhere[16,17] regarding the critical behavior of the conductivity do not depend on data obtained for the two samples closest to the transition.

Fitting the data for the 3.95×10^{18} cm^{-3} sample to Eq. (1a) yields a negative value for $\sigma(0)$, implying that this sample is insulating. For dopant concentrations just below the critical concentration the conductivity is expected to exhibit Mott[30] variable-range hopping of the form $\sigma(T)=\sigma_0\exp[-(T_0/T)^{1/4}]$. The conductivities are shown for several samples just below and just above the critical concentration plotted as a function of $T^{-1/4}$ on a semilogarithmic scale in Fig. 6. A crossover to insulating behavior is apparent as the dopant concentration is decreased, with the 3.95×10^{18} cm^{-3} sample clearly on the insulating side of the transition.

Table I lists the values of m and of the zero-temperature conductivity $\sigma(0)$, determined by fitting the low-temperature data to Eq. (1a). The zero-temperature conductivity is plotted as a function of boron concentration in Fig. 7, while Fig. 8 shows the coefficient m as a function of reduced concentration n/n_c using the value $n_c=4.06\times10^{18}$ determined for Si:B from the data as dis-

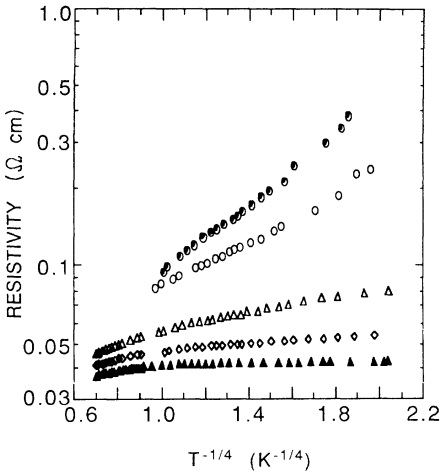

FIG. 6. The resistivity plotted on a logarithmic scale vs $T^{-1/4}$ for samples near the critical concentration, $n_c = 4.06\times10^{18}$ cm^{-3}. In units of 10^{18} cm^{-3}, the concentrations are as follows: ●, 3.90; ○ 3.95; △, 4.11; ◇, 4.20; ▲, 4.30.

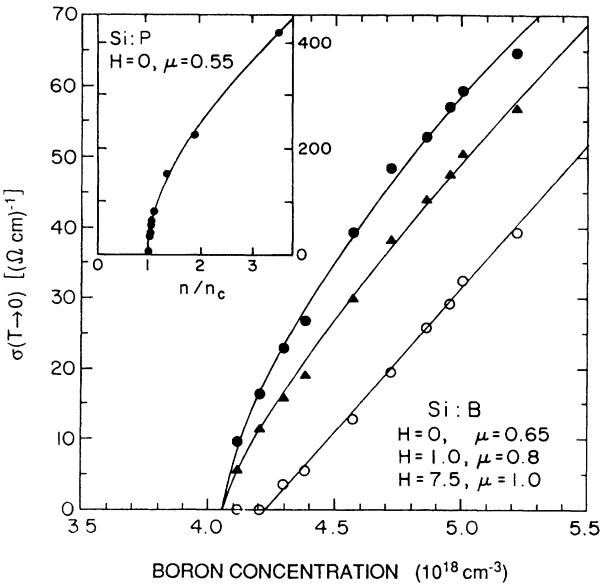

FIG. 8. The zero-temperature conductivity $\sigma(0)$ as a function of dopant concentration at $H=0$, $H=1$ T, and $H=7.5$ T. The lines represent fits to Eq. (7). The inset shows data for Si:P taken over a much broader range of concentration (see Ref. 2).

cussed later. Experimental values of m for Si:P (Refs. 2 and 3) and Si:As (Ref. 4) are also shown for comparison, and are quite comparable in magnitude and similar in behavior. Any small shifts along the horizontal axis may be associated with uncertainties in the determination of n_c. The coefficient m is given by the expression[23,24]

$$m=\alpha[(\tfrac{4}{3})-\gamma(3F_\sigma/2)]\ , \tag{2}$$

where $\alpha \propto (D)^{-1/2}$, D is the diffusion constant, and F_σ is an interaction parameter which will be discussed in more detail later. Bhatt and Lee[11] showed that γ depends sensitively in n-type material on the valley degeneracy, mass anisotropy, and the amount of intervalley scattering, with different conditions resulting in widely differing coefficients of the $T^{1/2}$ term. In particular, the magnitude of m can be explained in the case of Si:P if moderate anisotropy and no intervalley scattering is assumed. In the case of Si:B, however, the effects of anisotropy should be negligible, and intervalley scattering is not an issue. On the other hand, intervalence band scattering involving small momentum changes between the degenerate light- and heavy-hole bands is likely to have a significant effect. No theoretical calculations exist for this case. It is interesting to note that in spite of these differences, the experimental values of m are remarkably similar.

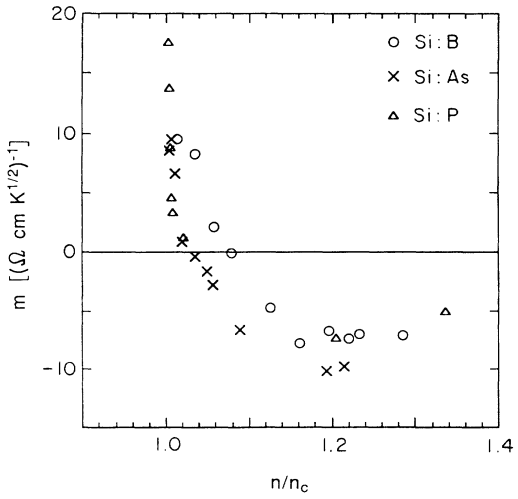

FIG. 7. The coefficients m deduced from fitting the data to Eq. (1a) plotted as a function of reduced concentration n/n_c, with $n_c = 4.06\times10^{18}$ cm^{-3} for Si:B. Also shown are the coefficients m for Si:P (Ref. 2) and Si:As (Ref. 3).

B. Temperature dependence of the conductivity in a magnetic field

A systematic investigation of the conductivity in various magnetic fields up to 7.5 T was carried out for all ten samples listed in Table I. The single most significant difference found experimentally between Si:B and Si:P is the sign of the magnetoresistance. In agreement with earlier results of Roth *et al.*[31] over a limited temperature range for a metallic sample further from the transition, we find that the magnetoresistance of Si:B is positive for all the boron concentrations we studied, at all temperatures and in all magnetic fields. In contrast, although the magnetoresistance[2,32] is predominantly positive in Si:P, a small negative component is found[2,32–34] at low fields due to single-electron localization. Thus, in the presence of spin-orbit scattering, the constructive interference between backscattered time-reversed paths which gives rise to localization becomes instead destructive interference or antilocalization. As demonstrated by Bergmann,[35] the dephasing by a magnetic field which contributes a negative magnetoresistance[36] in the case of localization yields instead of positive magnetoresistance[13,37] in the case of

antilocalization in the presence of spin-orbit effects. The absence of a negative component in the magnetoresistance of Si:B which is present in Si:P demonstrates that spin-orbit scattering has physically observable consequences for the behavior of its electrical transport.

Conductivities in various fixed magnetic fields between 0 and 1 T are shown as a function of $T^{1/2}$ in Figs. 9, 10, and 11 for three samples chosen such that their zero-field conductivities at low temperature have, respectively, negative, approximately zero, and positive slopes, $d\sigma/dT$. As in the case of zero or low field, we find approximately a $T^{1/2}$ correction to the conductivity at sufficiently high field, but with a different coefficient. For samples which are far from the transition, as in Fig. 9, the magnetic field causes the slope to change from negative to positive, while closer to the transition which m is already positive in zero field, it becomes even more positive, as in Fig. 11. The change in slope occurs at a temperature T_m which increases linearly with increasing field. Similar results have been obtained in Si:P by v. Lohneysen[38] and by Paalanen and Bhatt.[33]

The observed change in slope has been attributed to Zeeman splitting[1,39] in a magnetic field $g\mu_B H \gg k_B T$ which suppresses the diverging triplet channel amplitude which is responsible for the negative slope, leaving field-independent singlet channel contributions which give positive $T^{1/2}$ behavior. Since spin scattering mixes the spin-up and spin-down channels, it is also necessary that $g\mu_B H \gg \tau_{\text{s.o.}}^{-1}$ and τ_{Sp}^{-1}, where $\tau_{\text{s.o.}}$ and τ_{Sp} are the spin-orbit and spin-flip scattering times. The temperature of the maximum T_m is found experimentally to vary linearly with the magnetic field H. This implies that within the range of temperatures of these measurements, the first condition above, $g\mu_B H \gg k_B T$, governs the observed behavior and the spin-orbit and spin-flip scattering rates, both of which are expected to be independent of the temperature, are smaller than $k_B T$.

The maxima shown in Fig. 9 occur for Si:B at $H/T \approx 2.5$ T/K, which is within 10% or 15% of the values of H/T where maxima are found to occur in Si:P by Paalanen and Bhatt.[33] This is surprising, since the g value for Si:P is known to be very close to the free-electron value of 2, while $g = 1.2$ in Si:B.[14,15] It is puzzling that transport behavior which is governed by Zeeman splitting shows no evidence of this difference in the g values.

When $g\mu_B H \gg k_B T$ the conductivity is given by[1,39]

$$\sigma(H,T) = \sigma(H,0) + m' T^{1/2} , \tag{3}$$

with

$$m' = \alpha[(\tfrac{4}{3}) - \gamma(F_\sigma/2)] , \tag{4}$$

where the parameters are defined in connection with Eq. (2), and their range of values is such that m' is positive. Examination of Eqs. (2) and (4) indicates that a magnetic

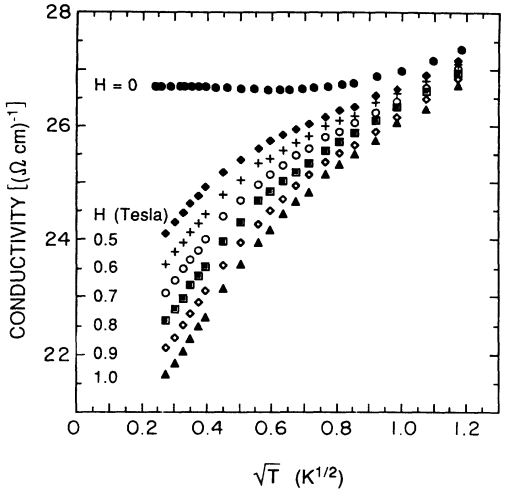

FIG. 10. Conductivity vs $T^{1/2}$ in magnetic fields between 0 and 1 T, as labeled, for Si:B with dopant concentration 4.38×10^{18} cm^{-3}.

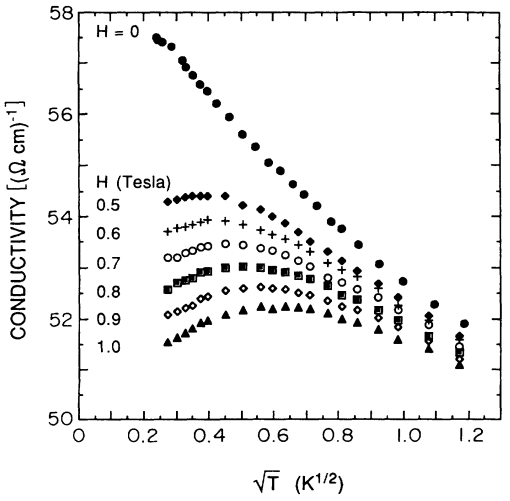

FIG. 9. Conductivity vs $T^{1/2}$ in magnetic fields between 0 and 1 T, as labeled, for Si:B with dopant concentration 5.01×10^{18} cm^{-3}.

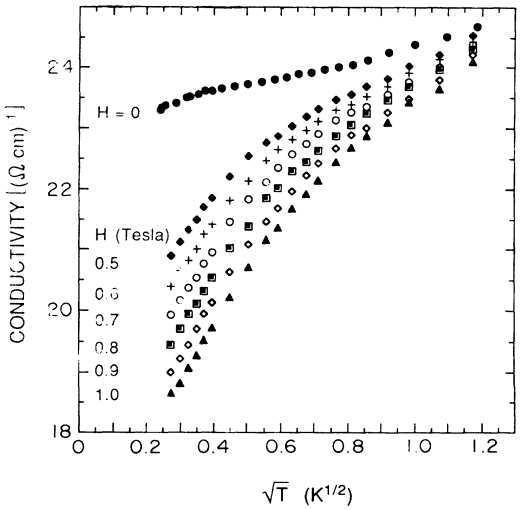

FIG. 11. Conductivity vs $T^{1/2}$ in magnetic fields between 0 and 1 T, as labeled, for Si:B with dopant concentration 4.30×10^{18} cm^{-3}.

field can cause a change in the slope whenever m in zero field is negative, namely in samples for which $\gamma F_\sigma > \frac{8}{9}$.

Figures 12 and 13 show the conductivity at low temperatures of all ten samples studied as a function of $T^{1/2}$ in fixed fields of 1 and 7.5 T. The data were fitted to Eq. (3), and the resulting values of m' and $\sigma(H,0)$ are shown as a function of boron concentration in Figs. 14 and 8, together with their zero-field counterparts. It should be noted that while the high-field condition $g\mu_B H \gg k_B T$ is only marginally satisfied at 1 T providing a limited range of temperature, a magnetic field of 7.5 T allows a fit over a fairly wide span. In contrast with the zero-field slope m which changes sign at $n \approx 1.08 n_c$, the slope m' is positive at 7.5 T, where $g\mu_B H > k_B T$ and, as seen in Fig. 14, it varies relatively slowly with concentration.

For the particle-hole channel, the contributions from interactions to the transport behavior as well as to the thermodynamic properties are determined by a single Fermi-liquid parameter F, the Fermi surface average of the screened electron-electron interactions. This dimensionless constant F which results from the Hartree interaction can be written as

$$F=(1/x)\ln(1+x)\ , \tag{5}$$

where $x=(2k_F/K)^2$, k_F is the Fermi wave number and K is the Thomas-Fermi screening wave vector. The screening length K^{-1} becomes very large near the transition, and one expects that F will therefore decrease toward zero as the transition is approached.

The parameter F_σ which appears in Eqs. (2) and (4) for m and m' above is related to the quantity F by[24]

$$F_\sigma=(-\tfrac{32}{3})[1-3F/4-(1-F/2)^{3/2}]/F\ . \tag{6}$$

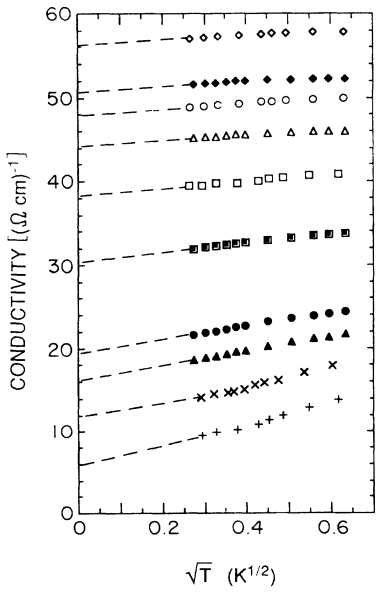

FIG. 12. The conductivity of ten Si:B samples in a fixed magnetic field of 1 T plotted against $T^{1/2}$ for temperatures below 0.5 K. In units of 10^{18} cm^{-3}, the dopant concentrations are as follows: +, 4.11; ×, 4.20; ▲, 4.30; ●, 4.38; ■, 4.57; □, 4.72; △, 4.86; ○, 4.95; ♦, 5.01; ◇, 5.22. The dashed lines are fits to Eq. (3).

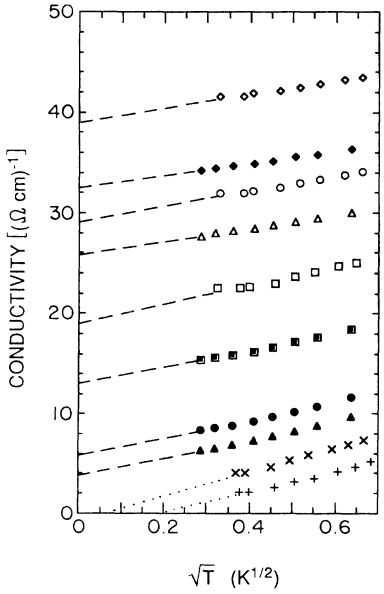

FIG. 13. The conductivity of ten Si:B samples in a fixed magnetic field of 7.5 T plotted against $T^{1/2}$ for temperatures below 0.5 K. In units of 10^{18} cm^{-3}, the dopant concentrations are as follows: +, 4.11; ×, 4.20; ▲, 4.30; ●, 4.38; ■, 4.57; □, 4.72; △, 4.86; ○, 4.95; ♦, 5.01; ◇ 5.22. The dashed lines are fits to Eq. (3). The dotted lines for the two lowest-concentration samples yield negative intercepts, indicating that these samples are in the insulating phase at 7.5 T.

Using the values determined experimentally for m in zero field and m' at 7.5 T, and assuming that neither γ nor the diffusion constant D which determines the coefficient α change when a magnetic field is applied, Eq. (2) and (4) can be used to determine the product γF_σ. The related quantity γF can then be computed for various assumed values of γ using Eq. (6).

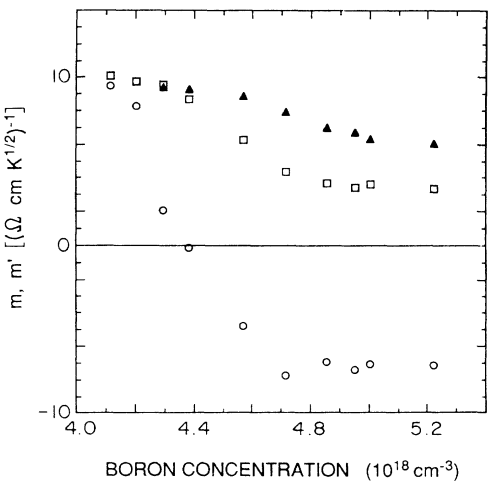

FIG. 14. The coefficients m deduced from fitting the data to Eq. (1a), and m' deduced by fitting the data in a magnetic field to Eq. (3), plotted as a function of dopant concentration n. The symbols denote the following: ○, zero magnetic field; □, 1 T; ▲, 7.5 T.

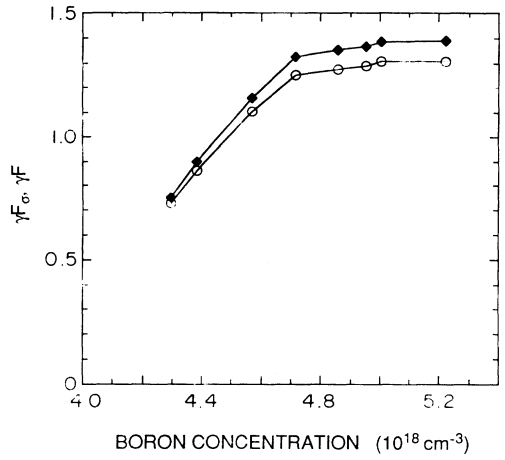

FIG. 15. The parameter γF_σ vs dopant concentration (closed diamonds). Also shown is the related quantity γF deduced through Eq. (6) for an assumed value $\gamma=2$ (open circles).

The values obtained for γF_σ are plotted in Fig. 15 as a function of dopant concentration. Also shown are the γF computed for the case $\gamma=2$. This choice of γ yields F's within the expected range between 0 and 1, and may be an appropriate value to take account of the heavy- and light-hole bands in Si:B. An informed choice for γ, however, awaits detailed theoretical work.

Few systematic investigations have been made to date of the concentration dependence of F. Studies by Bishop, Dynes, and Tsui[40] of the magnetoresistance in two-dimensional Si inversion layers yielded values for F as a function of $k_F l$ which were too high, and which increased rather than decreased as $k_F l$ was reduced. On the other hand, the change of sign of the slope m of the conductivity was attributed in Si:P (Ref. 2) and Ge:Sb (Ref. 7) to a diverging screening length and, through Eq. (5), a decreasing F as the transition is approached. As shown in Fig. 15, the values of F and F_σ calculated from our data for Si:B exhibit the expected decrease near the transition. One should bear in mind, however, that the validity of this analysis depends on the assumption that D and γ remain unchanged in a magnetic field. Further, the expressions for m and m' used to deduce F_σ were derived for weak disorder, so that it is by no means clear that the theory is applicable very near the transition.

C. The critical exponent

According to the scaling theory for disordered interacting electrons,[41] the critical behavior and universality class of a system are determined by symmetry-breaking fields such as spin-orbit effects, spin-flip scattering, or magnetic fields. Theoretical studies of the critical behavior of the coherence length yield a critical exponent $\nu=1$ for both the symplectic class corresponding to spin-orbit scattering,[42] and the unitary class for the case of a magnetic field.[41,43]

Experimental investigations of the critical behavior of the coherence length have largely been based on studies of the critical behavior of the electrical conductivity, obtained from determining the conductivity exponent μ in the expression.

$$\sigma(0)=\sigma_0[(n/n_c)-1]^\mu . \tag{7}$$

Here $\sigma(0)$ is the conductivity extrapolated to its value at zero temperature and n_c is the critical concentration for the transition.

For the case of pure localization with no interactions in three dimensions, the critical exponents μ and ν which characterize the behavior of the conductivity and of the coherence length are equal to each other at or near the transition. It is not clear that this remains true when electron correlations are important.[1] Further, the range of n/n_c for which this equality holds is not known or well understood. Nonetheless, the assumption has generally been made that $\nu=\mu$ over the entire range of concentrations measured, which in some experiments extends to twice the critical concentration.[2]

For essentially all the metal-semiconductor alloys, with the possible exception of amorphous Ar:Ga,[44] and for many doped crystalline semiconductors including uncompensated Ge:Sb,[8] the conductivity exponent is approximately equal to 1. The notable exceptions are the uncompensated n-type Si materials, namely Si:P,[2,3] Si:As,[4,5] Si:Sb,[6] and Si:P,As.[45] For these materials the conductivity exponent is smaller than 1 and close to $\frac{1}{2}$.[46] The only theoretical work which predicts an exponent of $\frac{1}{2}$ is by Hikami[47] for noninteracting electrons in the presence of spin-flip scattering. This does not give a satisfactory explanation for the anomalous exponent of $\frac{1}{2}$ in n-type uncompensated Si since studies of the conductivity have shown that interactions are important in these systems and must be taken into account. Spin-orbit or spin-flip scattering[33,46,47] have been mentioned as factors which may play a role. The suggestion has also been made that the change in sign which occurs in the slope $d\sigma/dT$ of the conductivity[33] may signal a crossover[48] between two different universality classes very near the transition which gives rise to an apparent rather than a real exponent different from 1. In any event, the anomalous exponent $\mu\approx\frac{1}{2}$ is not understood, and continues to be the focus of theoretical as well as experimental interest.

As discussed in more detail in the Introduction, spin-orbit effects are known to be important in Si:B.[12,13] The absence in Si:B of the negative component in the magnetoresistance which is found in Si:P indicates that spin-orbit scattering does indeed determine the sign of the single-electron (anti)localization contribution. Further, experimental evidence exists which indicates that the magnetoresistance becomes negative on application of uniaxial stress in Si:B (Ref. 49) and p-type germanium.[50] Since stress lifts the valence-band degeneracy which is responsible for the spin-orbit scattering, this is indeed what one expects.

Below we summarize our experimental findings[16,17] regarding the critical conductivity exponent in Si:B. Our results in zero field provide new information regarding the effect of spin-orbit scattering, while data at 7.5 T

TABLE II. Values of σ_0, the critical concentration n_c, and the exponent μ obtained from fits to Eq. (7) of the data at $H=0$, 1 T, and 7.5 T. Also listed for comparison are parameters for Si:P (Ref. 2) and Si:As (Refs. 3 and 4).

System	Magnetic field (T)	σ_0 $(\Omega\,\mathrm{cm})^{-1}$	n_c $(\Omega\,\mathrm{cm})^{-1}$	μ $(10^{18}\,\mathrm{cm}^{-3})$
Si:B	0	152^{+10}_{-18} $(=8\sigma_{\min})$	$4.06^{+0.12}_{-0.02}$	$0.65^{+0.05}_{-0.14}$
Si:B	1	155^{+12}_{-18}	$4.06^{+0.10}_{-0.03}$	$0.80^{+0.06}_{-0.14}$
Si:B	7.5	171^{+23}_{-25}	$4.22^{+0.12}_{-0.05}$	$1.0^{+0.10}_{-0.20}$
Si:P (Ref. 2)	0	260 ± 30 $(=13\sigma_{\min})$	3.74	0.55 ± 0.1
Si:As (Ref. 4)	0	376 ± 5 $(=16\sigma_{\min})$	8.58 ± 0.03	0.60 ± 0.05
Si:As (Ref. 5)	0	381	$7.8^{+0.3}_{-0.5}$	$0.64^{+0.20}_{-0.15}$

demonstrates the effect of a magnetic field on the critical behavior.

The conductivities extrapolated to their zero-temperature values as described in earlier sections are plotted in Fig. 8 as a function of dopant concentration. Data are shown for zero field, and in magnetic fields of 1 and 7.5 T. Two major important features are immediately apparent. One is the similarity of the zero-field, zero-temperature conductivity to that observed in Si:P,[2,3] where the exponent was found to have the anomalous value $\frac{1}{2}$. The other is the unmistakable change which occurs in a large magnetic field.

The coefficients σ_0, the critical concentrations $n_c(H)$, and critical conductivity exponents μ were obtained from nonlinear least-squares fits of the $\sigma(0)$ to Eq. (7) at zero field, at 1 and 7.5 T. The quoted errors for each parameter were obtained as follows. Using data for all measured concentrations, errors were first determined corresponding to one standard deviation with the other two parameters allowed to vary freely. As discussed earlier, however, the zero-temperature extrapolations become increasingly uncertain as the transition is approached, particularly for samples whose conductivity has a positive-temperature derivative at low temperature. For the data in zero field, the fitting procedure was therefore repeated as above, omitting data for the two samples closest to the transition. The error bars were then enlarged to include the possibility that only data for samples with a negative low-temperature slope are reliable.

The σ_0, n_c, and μ obtained from these fits at $H=0$, 1 T, and 7.5 T are listed in Table II. Also listed are experimental determinations of these quantities for Si:P (Ref. 2) and Si:As.[4,5]

We note that in the absence of a magnetic field the critical conductivity exponent is distinctly smaller than 1, and close to the value of $\frac{1}{2}$ found in Si:P. This in spite of the importance of spin-orbit effects which, as discussed earlier, give rise to a positive magnetoresistance. This finding implies that, contrary to expectations, spin-orbit scattering does not appear to determine the critical behavior of the conductivity in zero field. We suggest that the anomalous critical exponent of Si:B and of the n-type Si materials have a common origin which is still not understood.

The increase of n_c in a field of 7.5 T is presumably associated with field-induced modifications of the impurity wave functions. Most interesting is the change in the critical exponent μ toward the value 1, in agreement with the theoretical prediction. One should note that such a change can only be demonstrated for a material which has an exponent different from 1 in the absence of a field, as in Si:B, Si:As, or Si:P. To our knowledge, this is the first clear experimental demonstration of a change in universality class at the metal-insulator transition due to the application of a magnetic field.

IV. SUMMARY AND CONCLUSIONS

The properties of acceptors as compared with donors in silicon are determined in part by the character of the valence bands as compared with the conduction band. In n-type silicon, one needs to consider the effects of valley degeneracy, anisotropic mass, and of intervalley scattering. In the case of acceptors, complexities arise instead from the presence of the heavy- and light-hole valence bands. Further, while spin-orbit scattering is important in n-type silicon only for large mass donors, spin-orbit effects are associated in p-type material with the nature of the valence bands themselves, and are therefore always significant.

Despite these differences, the behavior of Si:B is found to be quite similar in many respects to Si:P and Si:As. The corrections to the zero-temperature conductivity due to the electron-electron interactions are comparable in size and similar in their dependence on reduced dopant concentration. The temperature dependence of the conductivity in fixed magnetic fields is also quite similar for Si:B and Si:P. Most significantly, the critical conductivity exponent in zero magnetic field has the same anomalous value near $\frac{1}{2}$ for Si:B as it does in n-type silicon, in spite of the strong spin-orbit effects associated with the valence bands.

The one important experimental difference between the two materials is the sign and size of the magnetoresis-

tance. While there exists a negative component in the magnetoresistance associated with single-electron localization in Si:P, the magnetoresistance of Si:B is positive for all measured concentrations, temperatures, and magnetic fields, indicating that the single-electron contribution derives from antilocalization due to spin-orbit scattering. It is also interesting to note that the magnetoresistance is much larger in Si:B than in Si:P, presumably due in part to the fact that the contributions associated with localization and interactions add in the former and oppose in the latter. This establishes a clear role for spin-orbit scattering in determining the transport behavior in Si:B. It is therefore intriguing that spin-orbit scattering has little apparent effect on the temperature-dependent corrections both with and without a magnetic field or on the critical conductivity exponent in zero field.

ACKNOWLEDGMENTS

The ion implants needed to make electrical contact to the Si:B samples were carried out at AT&T Bell Laboratories by Alice White. We thank her for her generous and invaluable contribution. We also wish to thank O. Entin-Wohlman, D. Schmeltzer, S. Sachdev, and M. Levy for valuable discussions. This work was supported by the U. S. Department of Energy under Grant No. DE-FG02-84ER45153. Partial support was also provided by the Professional Staff Congress, City University of New York.

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