

Conductivity of metallic Si:B near the metal-insulator transition: Comparison between unstressed and uniaxially stressed samples

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The low-temperature dc conductivities of barely metallic samples of p -type Si:B are compared for a series of samples with different dopant concentrations, n , in the absence of stress (cubic symmetry), and for a single sample driven from the metallic into the insulating phase by uniaxial compression, S . For all values of temperature and stress, the conductivity of the stressed sample collapses onto a single universal scaling curve, $\sigma(S, T) = \sigma_0 (\Delta S/S_c)^\mu G[T/T^*(S)]$, with $T^* \propto (\Delta S)^{z\nu}$. The scaling fit indicates that the conductivity of Si:B is $\propto T^{1/2}$ in the critical range. Our data yield a critical conductivity exponent $\mu = 1.6$, considerably larger than the value reported in earlier experiments where the transition was crossed by varying the dopant concentration. The larger exponent is based on data in a narrow range of stress near the critical value within which scaling holds. We show explicitly that the temperature dependences of the conductivity of stressed and unstressed Si:B are different, suggesting that a direct comparison of the critical behavior and critical exponents for stress-tuned and concentration-tuned transitions may not be warranted. [S0163-1829(99)14427-8]

I. INTRODUCTION

A continuous metal-insulator transition in the limit of zero temperature has been demonstrated over the past two decades since the pioneering results of Rosenbaum *et al.*¹ in a wide variety of disordered electronic systems, including uncompensated and compensated doped semiconductors, amorphous metal-insulator mixtures, and magnetic semiconductors. The region near the transition has been studied by tuning through the transition using the standard method of varying the concentration of one of the constituents¹⁻¹⁰ by uniaxial stress,^{11,12} using a magnetic field¹³ to vary the critical point, or using persistent photoconductivity to vary the doping in shallow levels.¹⁴

In metal-semiconductor mixtures and compensated semiconductors [including the persistent photoconductor, doped $\text{Al}_x\text{Ga}_{1-x}\text{As}$ (Ref. 14)] the onset of the conductivity is found to be well described by a particularly simple form in the metallic phase:

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

where $\sigma(t, 0) = A(t - t_c)^\mu$ is the zero-temperature conductivity, the critical conductivity exponent $\mu \approx 1$, and the coefficient B of the temperature-dependent term is independent of the tuning parameter t (the metal fraction, dopant concentration, stress, magnetic field, photoinduced carrier density, etc.) as it approaches the critical value t_c at the metal-insulator transition. Measurements of the conductivity for different values of t are thus found to yield a set of parallel straight lines when plotted against $T^{1/2}$.

Near a continuous zero-temperature phase transition governed by a quantum critical point, the critical behavior is expected to obey a standard scaling formalism.¹⁵ In particu-

lar, for a metal-insulator transition, the conductivity in the vicinity of the transition ($t \rightarrow t_c$, $T \rightarrow 0$) is expected to scale as

$$\sigma(t, T) = \sigma_c(T) f[(t - t_c)T^{-1/z\nu}], \quad (2)$$

where $\sigma_c(T) \propto T^{\mu/z\nu}$ is the temperature-dependent conductivity at $t = t_c$, μ is the exponent of the zero-temperature conductivity $\sigma(t, 0) \propto (t - t_c)^\mu$, ν is the exponent of the divergent correlation length $\xi \propto (t - t_c)^{-\nu}$, and z is the dynamical exponent relating spatial and temporal scales near the critical point $\tau \propto \xi^z$, with the characteristic temporal scale at a temperature T given by $\hbar/k_B T$.

By recasting Eq. (1) as

$$\sigma(t, T) = BT^{1/2} [1 + A(t - t_c)^\mu / BT^{1/2}] \quad (3)$$

it is easily seen to be a special case of the scaling form [Eq. (2)] with the identification $\mu/z\nu = 1/2$; in conjunction with the experimentally determined value $\mu = 1$, this implies $z\nu = 2$.

In contrast, the situation in uncompensated doped semiconductors, such as Si:P, Si:B, and Ge:Ga, appears to be much more complicated, and there continues to be debate and controversy (see, e.g., Refs. 16–18) concerning the behavior of the conductivity near the metal-insulator transition. Far from the transition deep in the metallic phase, the conductivity clearly exhibits a $T^{1/2}$ dependence¹⁹ at low temperatures, in agreement with Eq. (1) and consistent with perturbative results for a weakly disordered metal.²⁰ The coefficient B is found to depend weakly on dopant concentration deep in the metal, in qualitative agreement with theoretical expectations.²¹ Closer to the transition, however, the dependence of B on concentration becomes rather marked, and actually changes sign from negative to positive as the transition is approached. The full scaling relation, Eq. (2), is

not satisfied if one includes in the analysis both negative and positive slopes B . [In fact, if the conductivity obeys Eq. (1) near the transition, then scaling requires that the coefficient B scale as a power of $(t-t_c)$, so that reversals in the sign of B are explicitly excluded.] In the region close to the transition where the temperature coefficient of the low-temperature conductivity is positive, even the form of the temperature dependence of the conductivity is not clearly established: it has been reported in different experiments as $\propto T^{1/2}$ and $\propto T^{1/3}$.²²

Very different critical conductivity exponents have been obtained in uncompensated Si:P, considered the prototypical doped semiconductor. A value $\mu=0.5$ was found in the classic experiments of Paalanen *et al.*¹¹ down to very low temperatures (below 5 mK), where uniaxial stress was used to tune the transition. In experiments where the transition was approached by reducing the dopant concentration, similar exponents near 0.5 were found in Si:P (Ref. 7) as well as a number of other uncompensated doped semiconductors, including Si:As,⁴ double-doped Si:P, As,⁵ and Ge:Ga.¹⁰ In contrast, Stupp *et al.*⁸ found $\mu=1.3$ in Si:P, and Shlimak *et al.*⁹ deduced $\mu=1$ for uncompensated transmutation-doped Ge:Sb. These large exponents were based on data in a narrow range of dopant concentration near the transition where the coefficient B of Eq. (1) is positive. Using dopant concentration to tune the transition, a prior study involving one of the present authors reported $\mu=0.65$ in Si:B, a material in which the impurity states are characterized by an angular momentum $J=\frac{3}{2}$ arising from spin-orbit coupling characteristic of the valence bands of semiconductors like Si, and where spin-orbit scattering has been found to be strong.⁶

We have recently reported¹² measurements of the conductivity in Si:B in the immediate vicinity of the transition. By applying a compressive uniaxial stress, S , along the [001] direction using a pressure cell described elsewhere,²³ we have driven a sample of Si:B from the metallic phase toward the transition, and mapped out the conductivity as a function of applied stress (S) and temperature (T) in the range $0.05\text{ K} < T < 0.5\text{ K}$. We find that the conductivity is described accurately by the scaling form given by Eq. (2) (with $t=S$) for a range of stresses which yield conductivities that obey Eq. (1) with a constant coefficient B . However, the critical conductivity exponent is found to be $\mu \approx 1.6$, considerably larger than the values around $\mu=0.5-0.7$ reported by many workers, including that reported earlier for Si:B,⁶ where the transition was approached by varying the dopant concentration.

In this paper, we describe in detail the measurements on the metallic side of the transition and compare results obtained on a sample subjected to uniaxial stress with those obtained earlier for a series of unstressed samples in Ref. 6. We are led to the surprising conclusion that the two do not agree in detail, suggesting that further investigation of the issue of critical behavior in the presence of uniaxial stress is warranted. We describe the experimental details and results below, followed by a discussion and summary.

II. EXPERIMENTAL DETAILS AND RESULTS

A bar-shaped $8.0 \times 1.25 \times 0.3\text{ mm}^3$ sample of Si:B was cut with its long dimension along the [001] direction. Relatively

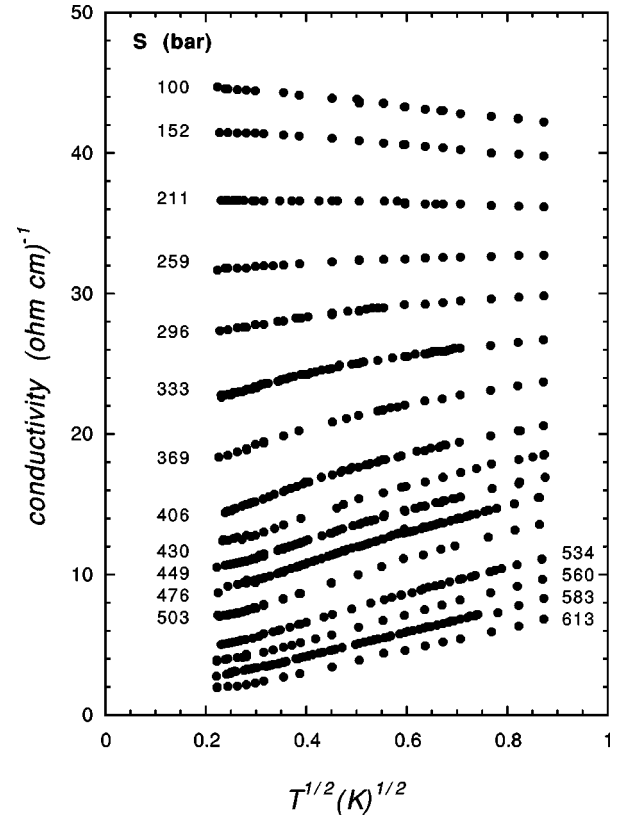


FIG. 1. Conductivity of Si:B versus $T^{1/2}$ for different values of uniaxial stress that place the sample in the metallic phase. The critical stress for this sample is 613 bar.

small uniaxial stress has a pronounced effect on the conductivity of Si:B, driving it initially toward more insulating behavior. A detailed discussion of the effect of stress is contained in a companion paper. The dopant concentration, determined from the ratio of the resistivities²³ at 300 K and 4.2 K, was $4.84 \times 10^{18}\text{ cm}^{-3}$. Electrical contact was made along four thin boron-implanted strips. Uniaxial compression was applied to the sample along the long [001] direction using a pressure cell described elsewhere.²³ Four-terminal measurements were taken at 13 Hz (equivalent to dc) for different fixed values of uniaxial stress at temperatures between 0.05 and 0.75 K. Resistivities were determined from the linear region of the I - V curves.

As discussed earlier, Eq. (1) is expected to be valid at low temperatures in the weakly disordered metal (perturbative regime),^{20,24} i.e., not too close to the transition. In the absence of theoretical predictions very near the transition, the conductivity is often fitted to this form everywhere, including the critical regime. Following this generally accepted procedure, we plot the conductivity of Si:B as a function of $T^{1/2}$ for various values of the stress S in Fig. 1. In agreement with experiments where dopant concentration is used to tune the transition, the slope B of the curves changes from negative to positive with increasing stress as the critical value S_c is approached. However, although the apparent straight-line behavior implies the validity of Eq. (1), an equally good fit (not shown) is obtained by plotting the data as a function of $T^{1/3}$. This method is therefore not sufficient to distinguish between the two functional forms.

We now present the results of a full scaling analysis of

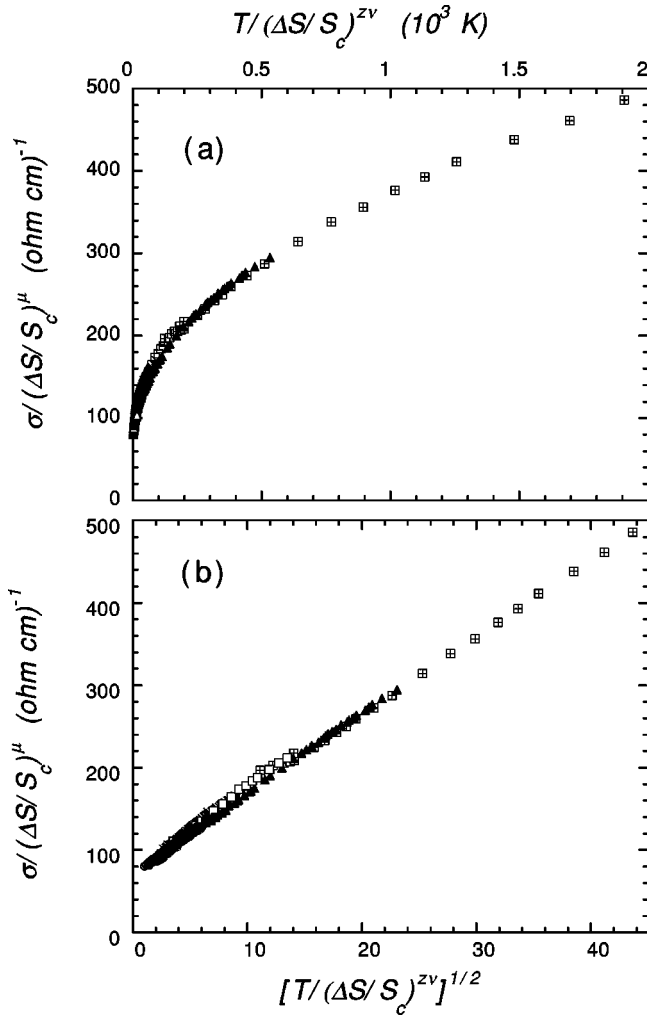


FIG. 2. (a) $\sigma(S,T)/(\Delta S/S_c)^\mu$ as a function of the scaling variable $T/(\Delta S/S_c)^{z\nu}$ with $\mu=1.6$ and $z\nu=3.2$ determined in Ref. 12. Here $\Delta S=(S-S_c)$, where S_c is the critical stress. (b) $\sigma(S,T)/(\Delta S/S_c)^\mu$ versus $[T/(\Delta S/S_c)^{z\nu}]^{1/2}$.

these data published elsewhere¹² and discuss its implications. The critical stress for the sample used in our experiments was determined to be $S_c=613$ bar; the temperature dependence at this value of stress, i.e., the critical conductivity, is $\sigma_c(T)\propto T^{0.5}$. We rewrite the scaling form, Eq. (2), as

$$\sigma(S,T)=\sigma(S,0)G[T/(\Delta S/S_c)^{z\nu}], \quad (4)$$

where $\Delta S=(S-S_c)$ and $\sigma(S,0)=\sigma_0(\Delta S/S_c)^\mu$. Guided by this version of the scaling form [Eq. (4)], the quantity $\sigma(S,T)/(\Delta S/S_c)^\mu$ is plotted in Fig. 2(a) as a function of the scaling variable, $T/(\Delta S/S_c)^{z\nu}$, with $z\nu=3.2$ and $\mu=1.6$ chosen to yield the best data collapse.¹² The resulting scaling function fully describes the temperature dependence of the conductivity in the conducting phase in the vicinity of the transition. If the usual assumption is made that $\mu=\nu$, then the dynamical exponent $z=2$, the same as that found in systems described by Eq. (1), such as semiconductor-metal mixtures and persistent photoconductors.

To test whether Eq. (1) provides a good description of the conductivity of Si:B very near the transition, we replot the same data as a function of $[T/(\Delta S/S_c)^{z\nu}]^{1/2}$ in Fig. 2(b). The data fall nearly on a straight line, indicating that the tempera-

ture dependence of the conductivity of Si:B just on the metallic side of the metal-insulator transition in the scaling regime is rather similar to that of metal-semiconductor mixtures and doped, highly compensated $\text{Al}_x\text{Ga}_{1-x}\text{As}$. This, in turn, implies that the $T^{1/2}$ corrections exhibited by the conductivity in the perturbative regime of the weakly disordered metal extend all the way to the critical point.²⁶ Pronounced failure of scaling occurs if we assume a critical temperature dependence in Si:B of $T^{1/3}$ instead of $T^{1/2}$; we are thus able to assert that the temperature dependence of the critical curve and the scaling function are decidedly inconsistent with the $T^{1/3}$ dependence that has been found in some other materials, such as Ge:Ga (Ref. 25) and Ge:Sb.⁹ Since Si:B and Ge:Ga are both acceptor systems, it would be of importance to see if similar scaling holds in the latter case, and whether the critical curve displays similar $T^{1/3}$ dependence.

A best straight line^{27,28} fit to the data of Fig. 2(b) yields

$$\sigma(S,T)/(\Delta S/S_c)^\mu=66+10.6[T/(\Delta S/S_c)^{z\nu}]^{1/2}. \quad (5)$$

Rearranging terms and making use of the fact that in our case $\mu=z\nu/2=1.6$, this can be written as

$$\sigma(S,T)=66(\Delta S/S_c)^{1.6}+10.6T^{1/2}, \quad (6)$$

where σ is in $(\Omega \text{ cm})^{-1}$ and T is in K. This is precisely of the form Eq. (1), as stated earlier.

A striking feature of these results is the very large critical conductivity exponent 1.6 compared to the exponent 0.65 found in earlier experiments⁶ where the transition was approached by tuning the dopant concentration. This is further illustrated in Fig. 3, which shows the zero-temperature conductivity of the stressed sample plotted as a function of $\Delta t/t_c$ on a linear scale compared with the conductivity obtained from a series of unstressed samples with varying dopant density. The symbols represent zero-temperature extrapolations obtained from the $T^{1/2}$ curves of Fig. 1 and the lower solid curve represents the first term on the right of Eq. (6); here the tuning parameter $t=S$. The upper solid curve represents the zero-temperature conductivity as a function of dopant concentration taken from Ref. 6; here the tuning parameter $t=n$. The difference between the results for stressed and unstressed samples is clear and dramatic.

To probe these differences further, we show in Fig. 4 the temperature dependence of the conductivities of a series of unstressed metallic samples close to the metal-insulator transition from Ref. 6 (shown as open circles) along with the data of Fig. 1. The two sets of data clearly do not overlap, as might be expected if tuning through the transition by varying stress or dopant concentration were equivalent. Although magnetic field-tuned transitions have long been recognized as different and belonging to a different universality class, it has generally been assumed that stress-tuned and concentration-tuned transitions are equivalent, allowing for direct comparisons of the critical behavior and critical exponents. The data of Fig. 4 seem to indicate that this is not the case. We discuss this point further in the next section.

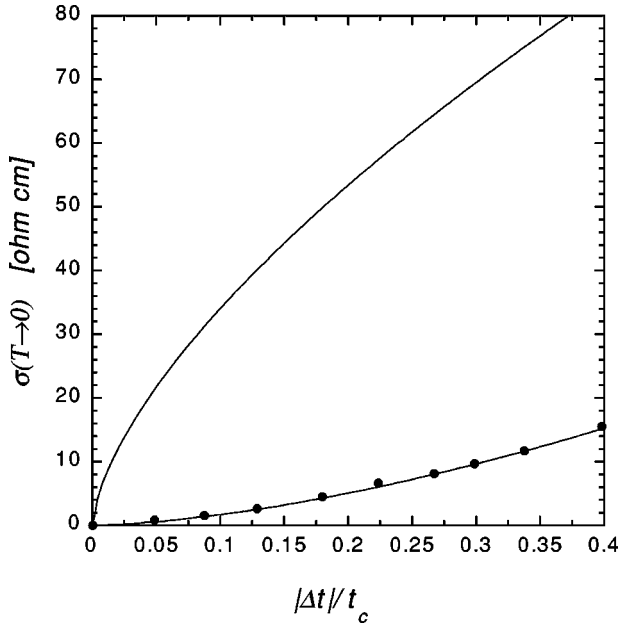


FIG. 3. The zero-temperature conductivity, $\sigma(T \rightarrow 0)$, versus $|\Delta t|/t_c$. The lower curve represents Eq. (3) with the parameters $\sigma_0 = 66 (\Omega \text{ cm})^{-1}$ and $\mu = 1.6$ found for the stress-driven transition (for which $t = S$); the symbols represent $T = 0$ extrapolations obtained from the temperature-dependent curves of Fig. 1. The upper curve, taken from Ref. 6, shows the critical behavior found earlier in experiments where the transition was approached by reducing the dopant concentration, $n = t$. Here $\sigma_0 = 152 (\Omega \text{ cm})^{-1}$ and $\mu = 0.65$.

III. DISCUSSION AND CONCLUDING REMARKS

The conductivity data in a metallic sample of Si:B subjected to a uniaxial stress along the [100] direction show clear evidence of scaling with temperature and stress as the metal-insulator transition is approached, in contrast with most previous data on uncompensated doped semiconductors. The scaling behavior enables one to determine with much more confidence the critical behavior at the transition, $\sigma_c(T) \propto T^{0.5}$, than is possible from the temperature dependence of individual samples. However, the scaling yields a much larger critical exponent $\mu \approx 1.6$ characterizing the zero-temperature conductivity, $\sigma(S, 0) \propto (S_c - S)^\mu$, than in the absence of stress.

This large difference naturally raises a number of questions. As stated earlier, acceptors in semiconductors are characterized by an angular momentum variable corresponding to $J = \frac{3}{2}$, and therefore have a fourfold degeneracy in the unstressed cubic crystal that is lifted in the presence of uniaxial stress. However, time-reversal symmetry, which is broken in the presence of magnetic field, is maintained in the presence of stress (the acceptor state is now twofold degenerate). Consequently, the change in universality class expected in the presence of a magnetic field is not expected for uniaxial stress. If, however, the breaking of the fourfold degeneracy leads to some (as yet unknown) new universality class, this effect should be easy to confirm experimentally—in Si:P, where there is no such degeneracy in zero stress, the unstressed and uniaxially stressed data should not have the large discrepancies seen in Si:B.

A potential source of error in the determination of the

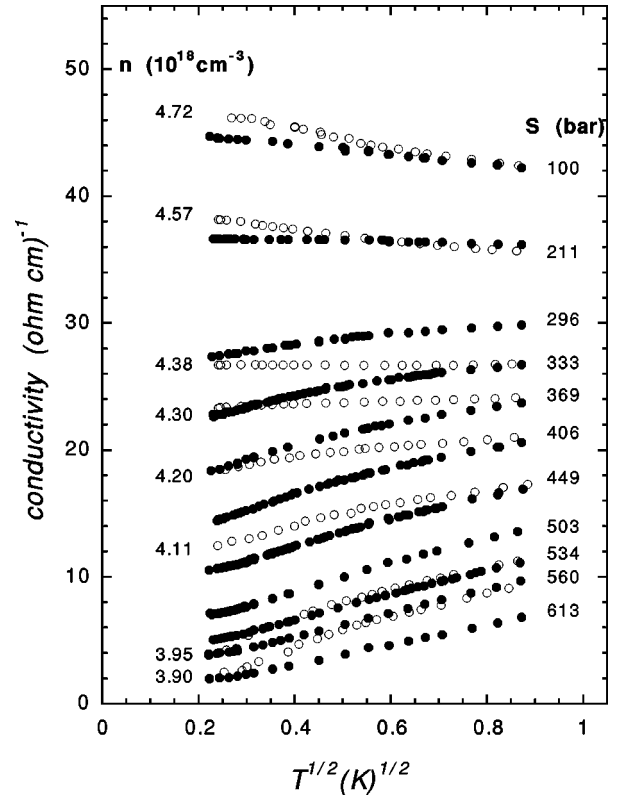


FIG. 4. The conductivity of stressed and unstressed Si:B plotted as a function of $T^{1/2}$. Closed circles denote data for a sample under stress and open circles indicate data for unstressed Si:B with different dopant concentrations as labeled.

critical exponent is strong nonlinearity in the stress dependence of the critical density. In both n - and p -doped Si (or Ge), the change in the critical density with stress can be attributed to a change in the impurity wave function.²⁹ In Si:P, the change at low stresses due to mixing of the central-cell split excited $1s$ states into the ground state can be calculated³⁰ and shown to be quadratic in S , i.e., $n_c(S) = n_c(0) - aS^2$. At large stresses, on the other hand, the impurity wave function is derived (for most directions of stress) from the two lowest conduction-band minima, and so the critical density $n_c(S)$ saturates as $S \rightarrow \infty$. As a result, $n_c(S)$ is a monotonic function of S , with an “S-shaped” curve, which can be reasonably approximated by a linear curve for small excursions around a critical value S_c , except for very small and very large S , the characteristic S corresponding to the strain given by the central cell splitting divided by the conduction-band deformation potential.

In Si:B, stress initially splits the $J = \frac{3}{2}$ acceptor state linearly, causing a much more dramatic dependence on the stress. A calculation of the acceptor wave function at low stress^{32,33} does not explain this large dependence; instead the predominant effect must come from the disappearance of the freedom to choose between orbitally distinct wave functions (as in the case of effective-mass donors³¹). For large compressive stresses along the [001] direction, on the other hand, the acceptor wave functions must be derived predominantly from the light-hole valence band, and therefore n_c is expected to decrease, as the acceptor wave function expands.^{32,33} Consequently, $n_c(S)$ actually exhibits a maximum as a function of S , so that an appropriately doped

sample of Si:B should exhibit a reentrant metal-insulator-metal transition as a function of stress.

In the absence of quantitative theory for $n_c(S)$, we base our assumption that nonlinearities are not significant on the experimental finding that both the stress dependence of the conductivity of our sample $\sigma(S, T)$ at a high temperature ($T=4.2$ K), and the dopant density dependence of the conductivity of a series of closely spaced unstressed samples $\sigma(n, T)$ at $T=4.2$ K, are *linear* in S and n , respectively, over the range of the control parameter around the critical value used in our analysis. Further, the critical stress for our sample, $S_c=613$ bar, lies well away from zero stress (where one might expect some complications from local strains due to a Jahn-Teller splitting of the acceptor state) and from the stress corresponding to the maximum resistivity at low T ($S_{\max}=3.5$ kbar), and is therefore less likely to be affected by nonlinearities in $n_c(S)$. Confirmation of this must await results on a series of samples with differing values of the critical stress S_c .

Another possible source for the unusually large exponent obtained in the current experiments is an inhomogeneous distribution of stresses resulting in a spread of ΔS 's and a consequent averaging over a distribution of conducting paths, some further and some closer to the transition. However, such a distribution might well be expected to give rise to measurable deviations from scaling, and the quality of the data collapse shown in Fig. 2 is excellent.

One also needs to consider possible effects associated with anisotropic conductivities in uniaxially stressed samples. For a sample under [001] stress, the conductivity along the stress direction $\sigma_l(S)$ differs from the conductivities along the transverse [100] and [010] directions, $\sigma_t(S)$. Assuming a normal Fermi liquid metallic phase, and since the critical stress S_c is nonzero, the conductivity anisotropy

$$\alpha(S) = 3[\sigma_l(S) - \sigma_t(S)] / [\sigma_l(S) + 2\sigma_t(S)] \quad (7)$$

may be expanded in an analytic Taylor expansion around S_c ,

$$\alpha(S) = \alpha(S_c) + (d\alpha/dS)_{S_c}(S - S_c), \quad (8)$$

which can easily be shown to lead to a subleading correction to the conductivity onset when measured in any direction, i.e., if we take

$$\sigma_{\text{tr}}(S) = [\sigma_l(S) + 2\sigma_t(S)]/3 = \sigma_0[(S_c - S)/S_c]^\mu \quad (9)$$

we obtain

$$\sigma_l(S), \sigma_t(S) \propto (S_c - S)^\mu [1 + O(S_c - S)], \quad (10)$$

where the coefficient of the term of order $(S_c - S)$ in the square brackets will be proportional to $(d\alpha/dS)_{S_c}$.

The anisotropy also affects the comparison between unstressed and uniaxially stressed samples shown in Fig. 4. In particular, one expects to be able to compare the stress dependence of the angle-averaged value $\sigma_{\text{tr}}(S)$ to the concentration dependence of $\sigma(n)$ of the unstressed (cubic) samples. Consequently, the longitudinal conductivities $\sigma_l(S)$ for the uniaxially stressed samples (closed circles in Fig. 4) should be divided by a stress-dependent anisotropy factor $[1 + 2\alpha(S)/3]$ when comparing with the unstressed samples. (In providing a direct comparison in Fig. 4, we have assumed

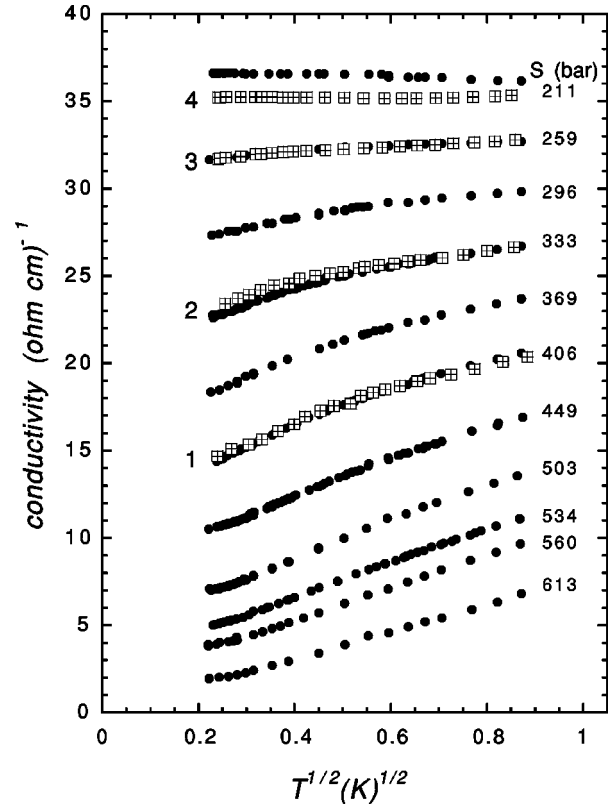


FIG. 5. Closed symbols denote the conductivity of stressed Si:B plotted as a function of $T^{1/2}$. The open square symbols represent the conductivity of four unstressed samples multiplied by an arbitrary factor $K = [1 + 2\alpha(S)/3]$ chosen to make them coincide with corresponding curves for the stressed samples, as follows: curves 1, 2, 3, and 4 denote $n = 4.11, 4.20, 4.30,$ and $4.38 \times 10^{18} \text{ cm}^{-3}$ with multiplicative factors $K_1 = 1.18, K_2 = 1.27, K_3 = 1.36,$ and $K_4 = 1.32,$ respectively; clearly, the unstressed curve at $n = 4.84 \times 10^{18} \text{ cm}^{-3}$ corresponds to $K = 1$.

that α is small at the stresses applied.) To test this, we multiplied each of the unstressed curves (open circles) by an arbitrary factor chosen to make it coincide with corresponding curves for the stressed samples. Our best attempt, shown in Fig. 5, requires rather large anisotropy values α ; moreover, the α 's (listed in the caption to Fig. 5) are unphysical: they are nonmonotonic functions of the stress, and decrease with increasing stress in the critical region. We therefore conclude that the difference between the temperature dependence of the uniaxially stressed and unstressed samples is intrinsic and not due to effects associated with anisotropic conductivities. Conclusive proof would require measurements of the conductivities in both the longitudinal and transverse directions in the presence of stress.

It should be noted that the scaling is found to hold only in a relatively small window of metallic conductivities for control parameter values rather close to the critical value. The much smaller exponent, $\mu \approx 0.5 - 0.7$, is derived from data over a much wider range. There has been much debate about the unusually small correlation length exponent ν that such a small μ implies, and possible violation of the bound derived for disordered systems $\nu \geq (2/d)$.³⁴ It is not clear whether such systems become inhomogeneous at long length scales and are then governed by percolation near the transition.³⁵ Such a scenario would offer the attractive possibility of rec-

onciling the many different results found in Si:P and Si:B. We point out that reports of large conductivity exponents^{8,12} are confined to a region very close to the critical value of the tuning parameter, where percolation may well result from such inhomogeneities. Further, the observed conductivity exponent is close to that expected for classical percolation in three dimensions.³⁶ Finally, this might account for earlier observations¹¹ of differing conductivities in different samples very close to the metal-insulator transition; the percolative paths could be rather sensitive to precise details of dopant distribution, and lead to nonuniversal amplitudes especially in a crossover region.

IV. SUMMARY

In summary, we have used compressive uniaxial stress applied along the [001] direction to approach the metal-insulator transition from the metallic side in Si:B. The conductivity scales with stress and temperature over the narrow range within which Eq. (1) is obeyed with a constant coefficient B . The temperature dependence of the conductivity at the critical value of the tuning parameter (uniaxial stress in our case) is found to be proportional to $T^{0.5}$. The critical exponent characterizing the onset of the zero-temperature conductivity is found to be $\mu = 1.6$, considerably larger than the exponent found in experiments where the transition was

approached by reducing dopant concentration. The temperature dependence of the conductivity is qualitatively and quantitatively different for stressed and unstressed Si:B, however, suggesting that a direct comparison of the critical exponents is not possible. Our data call for a systematic study of the stress tuned transition in other donor and acceptor systems, as well as for critical reexamination of the assumption that stress-driven and concentration-driven metal-insulator transitions are equivalent for all doped semiconductors.

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