COMMENTS

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Universality of the scaling exponents for the $T=0$ conductivity and Hall coefficient for very weakly compensated barely metallic silicon

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The critical behavior of the $T\rightarrow 0$ conductivity and Hall coefficient data is reexamined. Several "metallic" samples very close to n_c are found to fit Mott variable-range-hopping behavior expected for insulators. A slight increase in n_c for Si:P and Si:B results yields $\sigma(T\rightarrow 0)$ scaling exponents supporting universal behavior. The Hall results support scaling to a small value of n/n_c-1, but are currently inconsistent with a divergence of $R_H(T\rightarrow 0)$ as $n\rightarrow n_c$.

The stress-tuning results of Paalanen *et al.*[1] have established the standard for the prototypal uncompensated Si:P for determining the scaling behavior of $\sigma(n,T\rightarrow 0)$ by reaching lower temperatures (3 mK) than other groups. These authors obtained a conductivity exponent $s=0.51\pm 0.05$ with measurements in the range $0.0006<n/n_c-1<0.01$. Scaling data of very weakly compensated doped-Si systems has been obtained for Si:As,[2,3] Si:Sb,[4] Si:B,[5] and other Si:P studies,[6,7] although these studies have been on samples with a range of concentrations $n>n_c$. But, these studies have not reached as low temperatures, nor have they probed as close to n_c. These studies have all yielded values of s larger than the value of $\frac{1}{2}$ for Si:P, with these values ranging from 0.58 for Si:P to 0.65 for Si:B.[5] Following the pioneering Hall coefficient studies of Field and Rosenbaum[8] there have been Hall studies of the critical behavior of Si:As,[9] Si:B,[10] and Si:P.[11] These Hall studies all support the scaling of $1/R_H(T\rightarrow 0)$ as n approaches n_c, but these studies are not carried to as low temperatures as those in Ref. 1 and the question of whether R_H truly diverges at n_c is still not experimentally established. To date, there are no low-temperature uniaxial stress studies of the Hall coefficient to compare with the conductivity studies of Ref. 1. The Si results are reconsidered below and it is found that several samples for both Si:B (Ref. 10) and Si:P (Ref. 11) that are claimed to be metallic exhibit a temperature dependence that is a better fit to Mott variable-range hopping (VRH) over the temperature range of the data than to the $T^{1/2}$ behavior expected for the metallic side of the transition. This reconsideration demonstrates that the scaling behavior of σ for these systems yields exponents that are much closer to the $s\sim\frac{1}{2}$ value found in Ref. 1. These results strongly support the notion of universality for the metal-insulator transition (MIT) for these very weakly compensated Si systems. This is significant because the strong spin-orbit coupling for Si:B could lead to a different universality class (symplectic) for Si:B.

The most difficult aspect of experimentally determining accurate scaling exponents for the conductivity (Hall coefficient) is obtaining a reliable value of the critical density n_c. The approach of Paalanen *et al.*[1] was to obtain very low temperatures (3 mK) and with uniaxial stress and a single sample get very close to n_c ($n/n_c-1\sim 0.0006$). Even so, these authors did not attempt to analyze data with $\sigma<5$ S/cm and this regime is frequently termed the rounding region. In a recent effort to resolve the exponent puzzle question for Si:P, Stupp *et al.*[7] analyzed data in the vicinity of the rounding region and claimed a crossover to a larger exponent $s\sim 1.3$ very close to n_c, with the crossover occurring where $d\sigma/dT$ changes sign from negative to positive. These authors consider only the region with $d\sigma/dT>0$ to be the critical region. They also suggested a n_c for Si:P, which is 6% (a large change for critical behavior work) smaller than that obtained in Ref. 1. A recent analysis[12] of the temperature dependence of the data in Ref. 7 in the rounding region finds much better agreement with Mott VRH normally associated with insulating samples. The scaling of the Mott characteristic temperature T_0 with reduced density yields a value of n_c in excellent agreement with that in Ref. 1 and would make the crossover claim incorrect. The problem faced by experimentalists is that $d\sigma/dT>0$ in the critical regime for both barely metallic samples just above n_c and insulating samples just below n_c that exhibit Mott VRH behavior. It is just this problem that has led to values of n_c for the Si:B (Ref. 10) and Si:P (Ref. 11) that are smaller than obtained by the analysis given below, and which in turn lead to higher values of s than obtained for Si:P in Ref. 1.

In the Hall coefficient studies of Si:B and Si:P $1/R_H$

was plotted versus $T^{1/2}$. Several samples closest to n_c for each system (see Fig. 2 in Ref. 10 and Fig. 2 in Ref. 11) exhibit a temperature dependence that shows the slope of the $T^{1/2}$ term increasing steadily as the temperature is lowered. This is precisely the behavior that would be expected of samples obeying the Mott VRH law. In Fig. 1, this data is replotted as $\log R_H$ vs $T^{-1/4}$ for the Si:B 4.11 and 4.16 ($\times 10^{18}$/cc) samples and also for the Si:P 3.35 (Ref. 13) and 3.46 samples. Although there is some data scatter, the Si:B 4.11 and 4.16 are a better fit to Mott VRH than they are to the $T^{1/2}$ law. The Si:P results for the 3.35 and 3.46 samples are also a much better fit to the Mott VRH law than to the metallic $T^{1/2}$ law. If the data in Fig. 1 is fit to the result $R_H(T)=R_{H0}\exp(T_{0H}/T)^{1/4}$, one obtains for the Hall characteristic temperature T_{0H} the values 0.080 and 0.019 K for the Si:B 4.11 and 4.16 samples, respectively, while for Si:P one obtains 0.20 and 0.0187 K for the 3.35 and 3.46 samples. The Mott VRH behavior of $\sigma(T)$ yields Mott temperatures T_0 approximately a factor of 7 larger than T_{0H} very close to n_c at low fields, as shown for Si:As.[14] The present results are very similar to those for Si:As. The characteristic temperature T_{0H} scales as $n \rightarrow n_{c-}$ as

$$T_{0H}(n) \propto [1/N(E_F)\xi^3] = [1/N(E_F)\xi_0^3][(n_c-n)/n_c]^{3\nu}, \quad (1)$$

where $N(E_F)$ is the density of states at the Fermi level, ξ is the localization length, and ν is the localization length

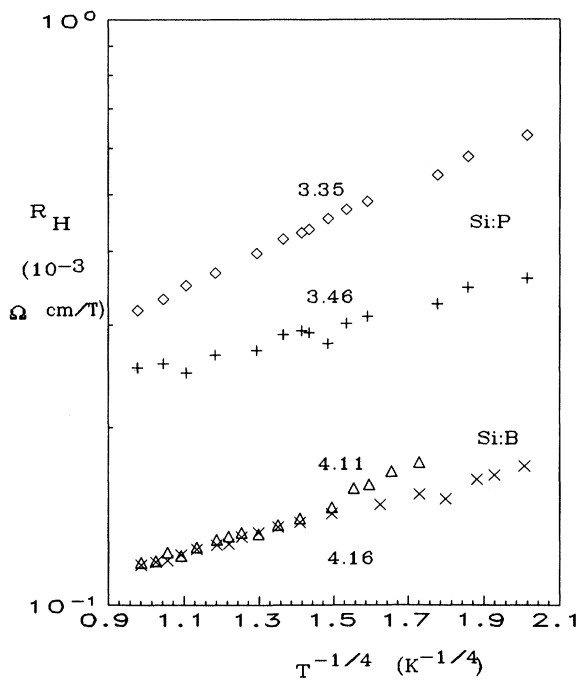

FIG. 1. The Hall coefficient $R_H(T)$ vs $T^{-1/4}$ for 3.35 (Ref. 13) and 3.46×10^{18}/cc Si:P and 4.11 and 4.16×10^{18}/cc Si:B samples. The data from Refs. 10 and 11 are a much better fit to the Mott VRH law than to the $T^{1/2}$ law expected for metallic samples.

scaling exponent. For insulating samples very close to n_c, the DOS in Eq. (1) is slowly varying and an expression for the ratio of two values of $T_{0H}(n)$ will be accurately approximated by

$$\frac{T_{0H}(n_1)}{T_{0H}(n_2)} \simeq \left[\frac{n_c-n_1}{n_c-n_2}\right]^{3\nu}. \quad (2)$$

Using the above values for Si:P, one obtains $n_c=3.532$ for $3\nu=2.54$ and $n_c=3.522$ for $3\nu=2.30$. The values of 3ν are in the same range as found for Si:As, where n_c has been reliably determined from scaling results of several physical quantities on both sides of the MIT. The same analysis for Si:B yields $n_c=4.225$ for $3\nu=2.54$. It is worth emphasizing that n_c is relatively insensitive to the value of ν, which is expected to fall between 0.6 and 1.0, but for Si:As is near 0.7. This simple way of obtain n_c from Mott VRH data has worked very well on the data of Stupp *et al.*[7] to confirm a value of n_c for Si:P in agreement with the original value obtained in Ref. 1. It is difficult to justify calling samples metallic (or at n_c) if they are a very good fit to the Mott VRH law. The traditional view has been that such samples are insulating, although it is sometimes claimed that this is not really Mott VRH when $T > T_0$. Alternatively, one would have to argue that n_c is itself a function of temperature, even when $T < 0.1$ K. For the Si:P results of Ref. 11, the present analysis increases n_c by 1.7% to 3.52 for the smallest value of 3ν. This is just at the upper limit of the error bars for n_c stated in Ref. 11. However, even this small change in n_c does have a significant effect on the magnitude of the conductivity scaling exponent s. For the Si:B case, two samples claimed to be metallic in Ref. 10 appear insulating because of their good fit to Mott VRH and this analysis then raises n_c by 4% for Si:B. Dai, Zhang, and Sarachik[5] have noted the 4.11 and 4.20 points in Ref. 5 are uncertain because of the possibility of a $T^{1/3}$ dependence and have given enlarged error bars $s=0.65\pm^{0.05}_{0.14}$ and $n_c=4.06\pm^{0.12}_{0.02}$. However, the $T^{1/3}$ dependence for $n > n_c$ should only be observed when $m(n)T^{1/2} > \sigma(n,0)$, which is not the case for the 4.11 and 4.20 samples. Furthermore, both of these samples show an increase in slope $m(n)$ (see Fig. 2 in Ref. 5) as T is reduced. The viewpoint espoused in the pioneering work[1] on Si:P was that extremely low temperatures were required as one approached n_c and this implies that only ultralow temperatures will produce accurate results in determining n_c. The results for Si:As (Ref. 2) and the above analysis suggest an alternative approach for accurately determining n_c, hence the question of accurately determining n_c deserves further discussion.

If one only relies on conductivity data to force fit the scaling expression $\sigma(n,T\rightarrow0)=\sigma_0(n/n_c-1)^s$, one is faced with determining three separate parameters, two of which (n_c and s) are strongly coupled. Moreover, one has already assumed the theoretical form to fit the data without being certain that a more complex expression for $\sigma(n,T\rightarrow0)$ can be ruled out. Stupp *et al.*[7] suggest a more complex fit although Ref. 12 disputes this fit. On the insulating side of the transition, both the dielectric

susceptibility $\chi'(n,T\rightarrow 0)$ and the Mott characteristic temperature T_0 (and T_{0H}) scale to infinity and zero, respectively, considerably faster than the conductivity on the metallic side. However, obtaining the asymptotic $\chi'(n,T\rightarrow 0)$ is as difficult or more difficult as for $\sigma(n,T\rightarrow 0)$ on the metallic side. While the Mott VRH characteristic temperature $T_0(n)$ $[T_{0H}(n)]$ can be determined accurately at higher temperatures, one faces a situation close to n_c where $\sigma(n<n_c,T)$ changes only by a small amount (less than one decade) and whether this is sufficient to accurately describe the conductivity as $T\rightarrow 0$. The generally expected behavior for a sample exhibiting Mott VRH at higher temperatures is that it will cross over to Efros-Shklovski VRH. (The Mott exponent of $\frac{1}{4}$ is replaced by $\frac{1}{2}$.) However, this only occurs for $T<T_0/1000$ and close enough to n_c $T_0<1$ K and the crossover is unreachable. Moreover, the extrapolation of Mott VRH results into the regime where $T_0<T$ has not yet been widely accepted. Nevertheless, the Si:As results[2] and the recent Si:P results[7,12] both show a dependence of T_0 on reduced density as T_0 scales to zero that yields a critical density $n_c$in excellent agreement with all other determinations for Si:As and in excellent agreement with the Si:P results[1] contrary to the view expressed in Ref. 7. For the Si:As case, the scaling data from two different quantities for $n>n_c$ and two other quantities for $n<n_c$ leads to $8.55<n_c<8.60\times 10^{18}$/cc. The minimum in the electron spin resonance (ESR) linewidth for Si:As occurs at 8.57 ± 0.04. This good agreement was obtained without the extremely low temperatures employed in Ref. 1. Significantly, the zero stress VRH data for both Si:P and Si:As is in excellent agreement with pure Mott VRH where "pure" implies a constant prefactor σ_0, which happens to be density independent for some range of density below n_c. This pure Mott VRH with no temperature-dependent prefactor then gives one confidence that the T_0 values obtained from a small range of $\sigma(T)$ values are reliable, providing accurate data is a very good fit to VRH behavior. Assuming this to be the case, this then suggests that the scaling of $T_0(n)$ leads to a more reliable determination of n_c than can be obtained from an arbitrary series of samples assumed to be metallic. This is precisely the problem faced in Refs. 6, 7, 10, and 11 where a group of samples, some insulating some metallic, were force fit to the $T^{1/2}$ behavior expected for metals, but employing temperatures that were more than an order of magnitude larger than the 3 mK used in the pioneering Si:P work.[1]

In Fig. 2(a) the scaling of $\sigma(n,T\rightarrow 0)$ is shown versus n/n_c-1 for Si: As,[2] Si:P,[11] and Si:B (Ref. 10) using the higher values of n_c obtained above. The earlier analysis[2,9] of Si:As was fit over too large a range of reduced density, beyond the scaling range of $R_H(n,T\rightarrow 0)$. For Si:As n_c has been increased only a small amount, but the maximum of n/n_c-1 has been reduced to 0.21. This has the effect of reducing the $\sigma(n,T\rightarrow 0)$ scaling exponent s from 0.60 ± 0.05 to 0.53 ± 0.05. The increases in n_c for Si:P and Si:B reduce s from 0.58 to 0.50 for Si:P and from 0.65 to 0.51 for Si:B. It is worth emphasizing that a 1% decrease in n_c for Si:B yields a 10% increase in

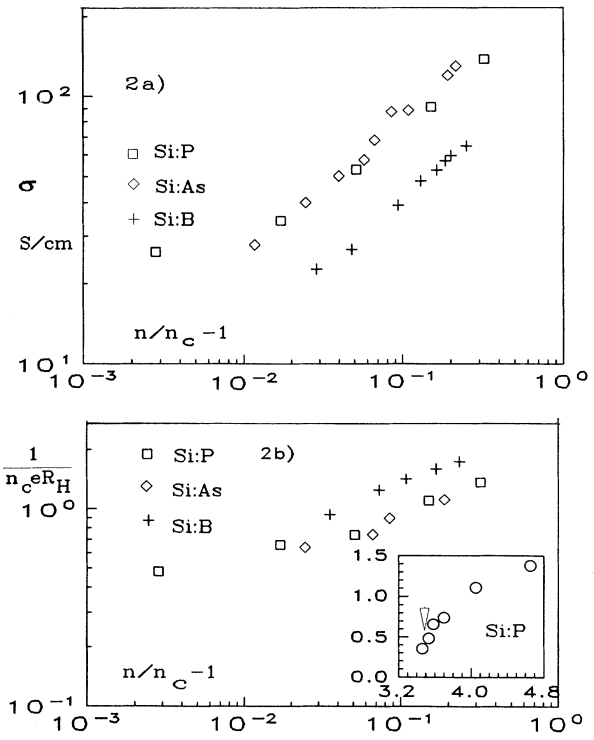

FIG. 2. (a) The conductivity $\sigma(n,T\rightarrow 0)$ vs reduced density n/n_c-1 for Si:P, Si:As, and Si:B. The n_c values employed are 3.52, 8.57, and 4.22×10^{18}/cc, respectively. Ignoring the flattening seen for Si:P the slopes yield scaling exponents 0.50, 0.53, and 0.51 with estimated errors of 10%; (b) the normalized reciprocal Hall coefficient $1/n_c eR_H(n,T\rightarrow 0)$ vs reduced density for the same values of n_c. The inset shows $1/n_c eR_H(n,T\rightarrow 0)$ vs donor density n. The arrow is centered at 3.49×10^{18}/cc and the width of the arrow ranges from $n_c=3.46$ used in Ref. 11 to the value of 3.52 in this work, which is the upper limit of the error range in Ref. 11.

s, thus demonstrating the importance of achieving very accurate values of n_c. A small flattening of $\sigma(n,T\rightarrow 0)$ is observed for Si:P in Fig. 2(a) at the smallest reduced density, which does not occur for the smaller $n_c=3.46$ used in Ref. 11. Since this lies at the heart of the difference in the two interpretations, we will return to this point. In Fig. 2(b) $1/en_cR_H(n,T\rightarrow 0)$ is plotted versus n/n_c-1 for the three Si cases employing the larger values of n_c. Within experimental uncertainties the Si:P (Ref. 11) and Si:As (Ref. 9) results are identical and lead to scaling exponents g equal 0.34 and 0.35, respectively, for $n>1.04n_c$. Both of these systems show a flattening at smaller reduced densities as $n\rightarrow n_{c+}$, which makes claims of a divergence of $R_H(T\rightarrow 0)$ untenable. Even if one employs $n_c=3.46$ for Si:P (as in Ref. 11) one still observes a flattening, but the onset of the flattening occurs at smaller values of reduced density. The inset in Fig. 2(b) shows $1/en_cR_H(T\rightarrow 0)$ vs n for Si:P (Ref. 11) and shows that this quantity would not approach zero until $n<3.40$. It is important to note that at n_c as interpreted in Ref. 11 the normalized $1/R_H$ is 0.36 of the classical value. As $n\rightarrow n_{c-}$ from the insulating side $T_{0H}\rightarrow 0$ and

TABLE I. $\sigma(n,T=0)$ and $1/R_H(n,T=0)$ scaling exponents.

	Current		New	
	s	g	s	g
Si:P	0.58	0.36	0.50	0.34
Si:As	0.60	0.355	0.53	0.35
Si:B	0.65	0.45	0.51	0.37

$R_H(T)\rightarrow R_{H0}$, a constant. This has been demonstrated for Si:As (Refs. 14 and 2) and illustrates the difficulty of getting $1/R_H(n>n_c,T\rightarrow 0)$ to scale all the way to n_c. The problem is a VRH contribution to $R_H(n\sim n_c,T)$ that is extremely difficult to remove with lower temperatures. The factor of 9 lower temperature reached in Ref. 11 compared to Ref. 9 is only a factor of 1.73 in $T^{-1/4}$. The Si:B results in Fig. 2(b) do not show a flattening as $n\rightarrow n_c$, but do show a flattening at larger n above $1.15n_c$, which is not surprising since $1/en_cR_H(n,T=0)$ must be 2 or less at $2n_c$ neglecting Hall correction factors. Figure 2(b) yields $g=0.37$ for Si:B below the flattening. Note that the normalized value of $1/R_H(T\rightarrow 0)$ at $n=1.035n_c$ is only 0.93 and is hardly strong support for a divergence of R_H.

Dai, Zhang, and Sarachik[11] argue that the results for Si:As would have shown no flattening if the results had been carried to lower temperatures. This is a possibility, but has not been firmly established in Ref. 11 since the 1.7% increase in n_c suggested in the present analysis produces the same flattening for Si:P as found for Si:As. Since this flattening is very sensitive to small changes in n_c, measurements to the 3-mk range of Ref. 1 may be required, but even 3 mK yields only a factor of 3.6 in $T^{-1/4}$ over that for 0.5 K reached for Si:As. Dai, Zhang, and Sarachik[11] caution that Hall results are much less accurate than conductivity results. This fact, combined with the greater difficulty of removing a VRH contribution from $R_H(T\rightarrow 0)$ than from $\sigma(T\rightarrow 0)$, suggests even 3 mK might be insufficient to totally remove the flattening. For n barely above n_c, it is reasonable to suppose that $1/R_H(T\rightarrow 0)$ is given by

$$1/R_H(n,T\rightarrow 0)=\lambda en_c(n/n_c-1)^g+1/R_{H,\,\mathrm{VRH}}\ , \quad (3)$$

where λ is a constant. The second term due to VRH could cause the flattening observed for Si:P and Si:As, however this has not yet been established experimentally. A new model[15] interprets the scaling term in Eq. (3) as yielding the mean density of free carriers $\langle n_{\mathrm{fc}}\rangle$ (averaged over the sample) in extended states and $n-\langle n_{\mathrm{fc}}\rangle$ as the mean density of localized states. The scaling of the Hall data demonstrates that for $n<1.01n_c$ one finds $\langle n_{\mathrm{loc}}/n\rangle>0.6$ for both Si:As and Si:P. The large density of localized states just above n_c makes it plausible that VRH could lead to the second term in Eq. (3), even on the metallic side of the transition. The potential importance of this VRH term in Eq. (3) illustrates the danger of force-fitting $1/R_H(T\rightarrow 0)$ data to a pure scaling form, particularly with the serious difficulties in accurately determining n_c from just "metallic" data.

Table I shows the current and the new values of the scaling exponents s and g for the three Si systems. The new s values are all within 6% of $\frac{1}{2}$, in much better agreement with earlier Si:P (Ref. 1) results, and make a much stronger case for the universality of the scaling of $\sigma(n\rightarrow n_c,T\rightarrow 0)$. The new Hall values of g exhibit more scatter, but appear to be approaching $\frac{1}{3}$. This is 33% below a theoretical value of $g=\frac{1}{2}$ obtained by Philips[16] by set theory. If one were to keep the current exponent values, then the case for universality would be substantially weakened. Since it is known the conductivity scaling exponent increases with compensation an alternative explanation for the larger values of s in Refs. 5 and 6 would be that these are not as weakly compensated as the earlier Si:P (Ref. 1) and Si:As (Ref. 2) samples. However, if one insists on the current, rather than the new n_c values then one must also explain why the temperature dependence of samples at n_c or just "metallic" is a much better fit to Mott VRH than to the $T^{1/2}$ dependence expected for the metallic side of n_c. Given the alternatives, the present analysis, which strongly supports universality, seems like the stronger case.

The importance of the spin-orbit (SO) coupling for isolated B acceptors in Si has been established by the ESR work of Feher, Hensel, and Gere.[17] In Ref. 5 it is argued the positive magnetoresistance for Si:B gives corroboration for SO scattering; however, both Si:P (Ref. 18) and Si:As (Ref. 19) also show very similar positive magnetoresistance contrary to the discussion in Ref. 5. In n-type Si it is well established that $\tau_{\mathrm{SO}}\gg\tau$ where τ is the elastic scattering time. The transport results to date for Si:B also suggest $\tau_{\mathrm{SO}}>\tau$. If SO scattering were dominant for Si:B it should be in the symplectic universality class. Castellani, Kotliar, and Lee[20] have obtained $s=1$ for this case. The results in Table I and the discussion in Ref. 5 suggest Si:B is in the same universality class as Si:P and Si:As.

In summary, evidence is presented showing certain metallic samples very close to n_c obey a temperature dependence in much better agreement with Mott VRH than with the expected metallic $T^{1/2}$ dependence, thus suggesting these samples are insulating. The n_c values for these Si:B and Si:P studies are enhanced slightly and this lowers the scaling exponents correspondingly. This analysis provides a good case for universality for the conductivity exponent s for Si:P, Si:As, and Si:B. On the other hand, the claims for a divergence of the Hall coefficient as $n\rightarrow n_{c+}$ are not consistent with the present data irrespective of which n_c value is selected. The overall evidence suggests the possibility of a VRH contribution to $1/R_H(T\rightarrow 0)$ in the immediate vicinity of n_c.

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