Possible Solution of the Conductivity Exponent Puzzle for the Metal-Insulator Transition in Heavily Doped Uncompensated Semiconductors

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The electrical conductivity σ (extrapolated to $T=0$) of uncompensated Si:P indicates a crossover as a function of P concentration N at N_{cr} slightly above the metal-insulator transition at N_c. For $N>N_{cr}$ the exponent of $\sigma\sim(N-N_c)^{\mu}$ is $\mu\approx 0.64$, while $\mu\approx 1.3$ for $N_c<N<N_{cr}$. At N_{cr} $d\sigma/dT$ changes sign from negative for $N>N_{cr}$ to positive for $N<N_{cr}$. σ in a magnetic field also yields $\mu\approx 1$. The apparent discrepancy between uncompensated and compensated semiconductors is traced back to a difference in the (nonuniversal) width of the critical region.

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The metal-insulator transition (MIT) is one of the key issues in the physics of disordered solids. Even in simple disordered systems like heavily doped semiconductors where the disorder stems from the statistical distribution of donor (or acceptor) atoms with concentration N in the single-crystalline host, the behavior of the electrical conductivity near the MIT occurring at N_c is not understood. [As usual, we denote a solid as metallic when the dc electrical conductivity σ remains finite for $T\rightarrow 0$, and as insulating when $\sigma(0)=\sigma(T\rightarrow 0)=0$.] Several investigations [1–8], notably on uncompensated semiconductors, have reported conductivity exponents μ close to 0.5, while $\mu=1$ for compensated semiconductors [9,10]. Here μ is defined by $\sigma(0)\sim(N-N_c)^{\mu}$. Amorphous alloys such as $Si_{1-x}Nb_x$ [11] show $\mu=1$ with the exception of Ar_{1-x}-Ga_x where $\mu=0.5$ [8]. This apparent classification of disordered solids into $\mu\approx 0.5$ and $\mu\approx 1$ without a clear physical distinction constitutes the "exponent puzzle."

Theoretically, $\mu=1$ is expected for noninteracting electrons for dimension $d>2$, based on an ε expansion around $d=2$, or on self-consistent calculations [12]. However, very close to the MIT this result may be questioned [12]. Also, electron-electron interactions become important. In a Fermi-liquid description the critical behavior depends on the presence (or absence) of symmetry-breaking fields [13]. Attempts have been made to invoke spin-orbit coupling as decisive for the critical behavior [14]. The lower bound $\mu=\frac{2}{3}$, based on the scaling law $\mu=\nu(d-2)$ where ν is the critical exponent of the correlation length, has been derived assuming one-parameter scaling [15]. Quite recently it was suggested that logarithmic corrections to scaling may mimic an apparent exponent $\mu\approx 0.5$ [16]. Also, quite unconventional approaches have been advocated [17].

In this situation more experimental work is needed, together with a critical assessment of existing experimental data. The main concerns are the following: (i) the extrapolation of the measured conductivity $\sigma(T)$ to $T=0$, (ii) the concentration determination, (iii) the determination of the critical concentration, (iv) possible sample inhomogeneities, and (v) the range of critical behavior. These problems are inherent in all the experiments (including the present one). In the very elegant stress-tuning experiment by Paalanen *et al.* [2], (ii) was circumvented by stress tuning N_c, i.e., forcing a given sample through the MIT by uniaxial stress. However, the other points still stand. In particular, concerning (iii), the problem was shifted to a determination of the critical stress S_c instead of N_c.

In the present work we present conductivity measurements on Si:P, together with a close analysis of the concerns raised above. Our data show a clear crossover of σ as a function of $(N-N_c)/N_c$. This crossover is related to the sign change of the temperature coefficient of $\sigma(T)$. Clearly, a MIT is only approached when $d\sigma/dT$ is positive, i.e., σ decreases with decreasing T. Hence the critical region is limited to the corresponding concentration region. In this region, which is very small for uncompensated Si:P, we find strong evidence for μ close to (actually a little larger than) 1, thus resolving the exponent puzzle. In addition, we present measurements on a barely metallic sample where magnetic-field tuning through the MIT also yields $\mu\approx 1$. The samples were all cut from the same Czochralski-grown rod (54 mm diameter) with a P concentration gradient of $N^{-1}(\Delta N/\Delta x)=10^{-2}$ cm^{-1}. The samples (typical dimensions $20\times 1\times 0.5$ mm^3, with the shortest axis parallel to the growth direction) were etched to avoid surface conductivity and contacted with Au wires by spark welding, with the voltage leads 8 mm apart. The resistivity at low T was measured with a standard four-point lock-in technique ($f=43$ or 218 Hz) in a contrast current mode with the power generated in the sample kept below 5×10^{-15} W.

A "preliminary" P concentration N_ρ was determined from the room-temperature resistivity ρ using the Thurber scale [18]. In order to exclude geometry errors, the resistance ratio $r=R(296\text{ K})/R(4.2\text{ K})$ was determined for $\sim$60 samples. A spline fit to the r vs N_ρ data yielded the P concentration N for a sample with measured r. The Hall concentration $N_H=(|R_H|e)^{-1}$ determined from the Hall coefficient R_H at 296 K yielded an r vs N_H dependence similar to r vs N_ρ, with the difference due to the Hall scattering factor. No significant difference when using both scales was found in the critical behavior of $\sigma(0)$ [19]. Macroscopic concentration fluctuations were smaller than 0.1% as checked by the varia-

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tion of r across the samples.

Figure 1 shows σ vs $\sqrt{T}$ for several samples close to the MIT. These data extend previous data obtained on different uncompensated Si:P samples [10,20,21] in one important aspect. Here, we report on about 10 metallic samples with $m = d\sigma/d\sqrt{T} > 0$ while the previous studies included only 3. Towards larger N (not shown) we observe $M = 0$ for a sample with $\sigma(0) = 60\ \Omega^{-1}\text{cm}^{-1}$ (corresponding to $N = 4.00\times10^{18}\ \text{cm}^{-3}$) and $m < 0$ for even larger N, as reported before [20–22].

Electron-electron interactions in disordered systems lead in lowest order to a correction $m\sqrt{T}$ to $\sigma(0)$ [23]. The negative m in Si:P for $N/N_c \gtrsim 1.2$ can be quantitatively accounted for [21,22]. However, the sign change of m close to N_c is not properly understood. Our data show that $\sigma(T) = \sigma(0) + m\sqrt{T}$ is approximately obeyed between $\sim$35 and 150 mK, and, furthermore, that m does not vary much for $N \to N_c$. The slight upturn at lowest T can be attributed to thermal decoupling of the Si:P samples from the cold source. Thus, although our data do not extend as low as previous data [1], the overall similar T dependence for our samples with different N makes the extrapolation to $T = 0$ rather unambiguous except for samples with $N \leq 3.52\times10^{18}\ \text{cm}^{-3}$.

Figure 2 shows $\sigma(0)$ vs N. In Fig. 2(a) the data are compared to a fit $\sigma(0) = \sigma_0[(N - N_c)/N_c]^{\mu}$ including all measurements up to $N = 7\times10^{18}\ \text{cm}^{-3}$ (see inset). This fit yields $N_c = 3.72\times10^{18}\ \text{cm}^{-3}$ and $\mu = 0.55$. The fit looks deceptively good, thus seemingly supporting $\mu \approx 0.5$. However, several objections arise. (i) The fit is actually best in the noncritical region far from N_c where $m < 0$. Only three data points are described by the fit for $m > 0$. (ii) The samples with $\sigma(0) < 20\ \Omega^{-1}\text{cm}^{-1}$ are not at all described by the fit. Such low-σ samples are usually discarded because of the "rounding" of the transition close to N_c. However, from the $\sigma(T)$ behavior (cf. Fig. 1) we find no significant difference from the higher-σ samples. (iii) The thermoelectric power S of the sample with $N = 3.58\times10^{18}\ \text{cm}^{-3}$ and $\sigma(0) = 3.3\ \Omega^{-1}\text{cm}^{-1}$ convincingly shows that this sample is metallic while a sample with $3.50\times10^{18}\ \text{cm}^{-3}$ with a divergence of S for $T \to 0$ was clearly insulating [24]. Metallic behavior of S was also established for $N = 3.54\times10^{18}\ \text{cm}^{-3}$ [25]. Thus N_c must be considerably smaller than the value inferred from the fit in Fig. 2(a).

Considering asymptotic critical behavior of $\sigma(0)$ only for $N < 4.00\times10^{18}\ \text{cm}^{-3}$ where $m > 0$, the resulting best fit [cf. Fig. 2(b)] for the critical exponent is $\mu = 1.3$, with $N_c = 3.52\times10^{18}\ \text{cm}^{-3}$. With this value of N_c, we show in Fig. 3(a) $\sigma(0)$ vs $(N - N_c)/N_c$. A clear crossover of $\sigma(0)$ is seen at $N_{\text{cr}} \approx 4.0\times10^{18}\ \text{cm}^{-3}$, which is indeed identical to the concentration where $M = 0$ [see Fig. 3(b)]. For $N > N_{\text{cr}}$ one obtains an *effective* exponent $\mu = 0.64$ close to the fit in Fig. 2(a). Classifying the sample with $N = 3.52\times10^{18}\ \text{cm}^{-3}$ as metallic [with $\sigma(0) \approx 0.5\ \Omega^{-1}\text{cm}^{-1}$, cf. dashed line in Fig. 1], no significant change of μ on both sides of N_{cr} would occur.

It has been suggested that $\sigma \sim T^{1/3}$ at N_c [26]. Plotting our data for samples close to N_c as σ vs $T^{1/3}$ to extract $\sigma(0)$, we found no significant difference in the crossover behavior of $\sigma(0)$ vs N. Below N_{cr} the critical ex-

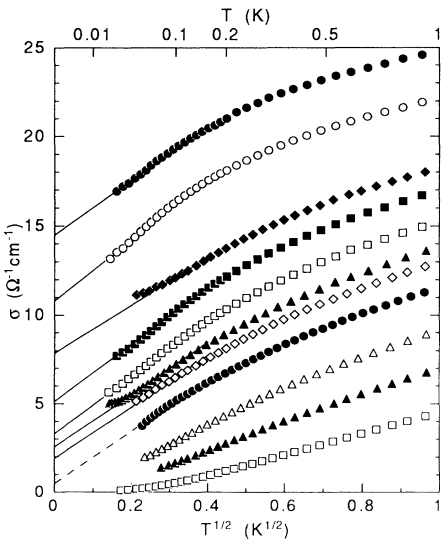

FIG. 1. Electrical conductivity σ vs square root of temperature $\sqrt{T}$ for Si:P samples with P concentration N close to the MIT. Solid lines indicate extrapolation to obtain $\sigma(0)$. The concentrations are (from top to bottom in units of $10^{18}\ \text{cm}^{-3}$): 3.69, 3.67, 3.63, 3.60, 3.58, 3.56, 3.55, 3.52, 3.50, 3.45, and 3.38.

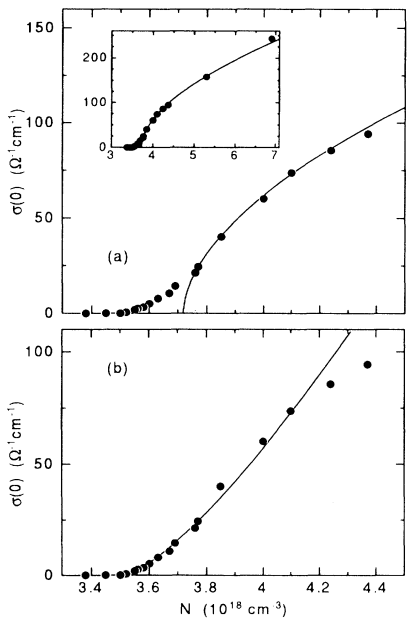

FIG. 2. Extrapolated conductivity $\sigma(0)$ for $T \to 0$ vs P concentration N. (a) Fit with $\mu = 0.55$, $N_c = 3.72\times10^{18}\ \text{cm}^{-3}$. Inset shows the same fit over an extended N range. (b) Fit with $\mu = 1.3$, $N_c = 3.52\times10^{18}\ \text{cm}^{-3}$.

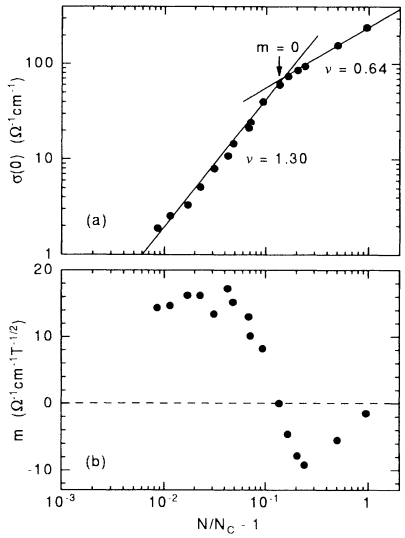

FIG. 3. (a) Extrapolated conductivity $\sigma(0)$ vs reduced P concentration $(N-N_c)/N_c$ with $N_c=3.52\times10^{18}$ cm^{-3}. (b) Coefficient m of the T dependence of σ vs $(N-N_c)/N_c$.

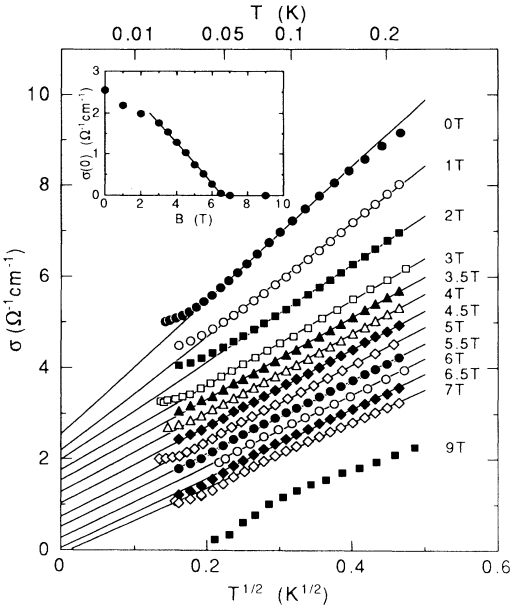

FIG. 4. Electrical conductivity σ vs $\sqrt{T}$ for Si:P with $N=3.56\times10^{18}$ cm^{-3} in magnetic fields B between 0 and 9 T. Solid lines indicate extrapolation to obtain $\sigma(0)$. Inset shows $\sigma(0)$ vs B.

ponent would become even larger, $\mu\approx1.6$.

All previous data on uncompensated semiconductors (with the exception of the stress-tuning experiment which will be discussed below) which purported to show $\mu\approx0.5$ actually relied on a fit such as the one shown in Fig. 2(a), i.e., putting much weight on data outside the critical region. For the published data [3–7] close to the MIT where $M>0$ a linear or slightly superlinear fit actually is often better. Occasionally, this was even noted by the authors themselves [5]. Allowing for a crossover one can consistently describe all existing conductivity data on uncompensated heavily doped semiconductors with $\mu\approx1$ for $N_c<N<N_{cr}$ and an effective exponent $\mu\approx0.5$ for $N>N_{cr}$, simply by choosing N_c accordingly. For the different systems the crossover occurs in all published data, when reanalyzed, at a concentration which is within a factor of 2 of the concentration where $m=0$.

We now compare our data with the stress-tuning results [2,27] on barely insulating Si:P samples which were forced into the metallic state by uniaxial pressure. For the determination of $\mu\approx0.5$ from these measurements, data for stress yielding $\sigma(0)<5\ \Omega^{-1}\text{cm}^{-1}$ were not included. The $\sigma(T)$ curves for these stresses showed a distinctively different behavior, with $\sigma=\sigma(0)+hT^2$ [instead of the $m\sqrt{T}$ correction to $\sigma(0)$] which had been already observed for samples very close to N_c, i.e., $(N-N_c)/N_c<0.01$ [1]. On the other hand, all our samples which we classify as metallic exhibit an approximate $\sqrt{T}$ behavior of σ (in an admittedly higher T range) as discussed above. The published [1] $\rho(T)$ curves ($2\text{ mK}\le T<100$ mK), which were extrapolated to yield a $\rho(0)$ of 0.6 and 1.4 Ωcm, above 50 mK can be interpreted as $\sigma=\sigma(0)+m\sqrt{T}$ with $\sigma(0)\approx0.6$ and $\approx0.1\ \Omega^{-1}\text{cm}^{-1}$, and $m=20$ and 13 $\Omega^{-1}\text{cm}^{-1}\text{K}^{-1/2}$, respectively, and a leveling off below 25 mK. The m values thus inferred are within the range of our data [cf. Fig. 3(b)]. Also the stress-tuning data for samples very close to the MIT differ somewhat for the two sets of measurements [2,27]. This is only to indicate that even if data are obtained at very low T, there is some ambiguity in the interpretation. However, there are major differences between our data and the earlier ones [27] in the same T range (160 to 30 mK) where, e.g., σ of our sample with $N=3.60\times10^{18}$ cm^{-3} decreases from 11 to 7.5 $\Omega^{-1}\text{cm}^{-1}$, while σ of a sample under 5.73 kbar decreases from 11 to 4 $\Omega^{-1}\text{cm}^{-1}$. These differences cannot be resolved at present. Therefore, it is essential to provide an independent check of whether a given set of samples is metallic. The thermoelectric power measurements [24,25] mentioned above convincingly place samples with $N\ge3.54\times10^{18}$ cm^{-3} on the metallic side of the MIT.

The magnetic-field dependence of $\sigma(T)$ of a barely metallic sample $N=3.56\times10^{18}$ cm^{-3} is shown in Fig. 4. $\sigma(T)$ follows the $\sqrt{T}$ behavior over an appreciable T range up to fields $B=6$ T. Again, the leveling off at lowest T is due to thermal decoupling. Data for $B\ge6.5$ T indicate that the sample has been pushed through the MIT. The inset of Fig. 4 shows the extrapolated $\sigma(0)$ vs B, displaying the MIT at $B_c=6.5$ T, with a critical exponent $\mu'=1$ from $\sigma\sim(B_c-B)^{\mu'}$, which is not too far from $\mu=1.3$ for $B=0$.

We can relate field and concentration scales by relating the roughly linear change of $\sigma(0)$ with B to that of $\sigma(0)$ with N, or by determining the change of N_c in a field of 6

T (not shown). Both methods yield $(\Delta N/N_c)/\Delta B \approx 5 \times 10^{-4}$ T^{-1}. Hence we are well in the critical region. Our observation $\mu \approx \mu'$ thus shows that the critical behavior appears to be independent of magnetic field.

The same conclusion with a critical exponent $\mu \approx 1$ close to N_c—independent of B—can be drawn for the system Si:B with strong spin-orbit scattering, when the above analysis assuming a crossover is applied. For $B=0$, only three samples in the critical region were investigated [7]. For these, $\sigma(0)$ vs N is actually perfectly linear [7]. Spin splitting in a magnetic field leads to a negative magnetoconductance and, more importantly in the present context, to a sign change of m for $g\mu_B B \gg k_B T$ [23]. This has been observed also in Si:P [21,22]. The sign change actually expands the critical region, thus allowing one to trace $\mu \approx 1$ over a larger set of samples. This difference in the width of the critical region, together with the (small) shift of N_c with field, explains in our view the large experimental differences for $B=0$ and $B \neq 0$ in Si:B [28].

A number of numerical investigations of an MIT driven purely by disorder (without interactions) have been performed yielding critical exponents $\mu \approx \mu' = 1.3$ to 1.5 independent of B [29–32]. Since these calculations probe metals rather close to the MIT, the agreement with our experimental result is significant.

In conclusion, we have shown that the zero-temperature conductivity of Si:P close to the MIT exhibits a crossover at N_{cr} which roughly coincides with the concentration where $d\sigma/dT$ changes from negative where the sample behaves as a "good" metal to positive, as required for a system approaching the insulating state. Since N_{cr} in Si:P is within 10% of N_c it is difficult to clearly separate this crossover from rounding effects very close to N_c. In the present work this has been possible through the study of a large number of metallic samples with $N_c < N < N_{cr}$. For these samples we observe a critical conductivity exponent $\mu = 1.3$, close to μ found for compensated samples. The difference to the latter lies therefore primarily in the nonuniversal ratio N_{cr}/N_c. We speculate that it is due to the difference in the relative contributions of disorder and electron-electron interactions to the behavior of σ close to N_c. It is hoped that our results will stimulate more theoretical work along these lines which is highly needed for a complete understanding.

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