Sharp Metal-Insulator Transition in a Random Solid

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Zero-temperature metallic conductivities have been measured above and below Mott's minimum value σ_{min} in bulk crystals of P-doped Si. Conductivities below σ_{min} increase by over 10^3 as the density is raised by less than 1%, and do not rule out a discontinuous transition. However, over a wider density range the data can be fitted with a scaling form with a characteristic length that tends to diverge with the same exponent in the metal and insulator.

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In 1972, Mott[1] proposed the existence of a finite minimum conductivity σ_{min} at zero temperature and frequency in a metallic three-dimensional random system. The idea was based on the Ioffe-Regel criterion[2] that for metallic behavior the electron's mean free path must exceed its wavelength, and on Anderson's prediction[3] that, for a certain value of the disorder, states become localized. The value of σ_{min} is given by a constant times $e^2/\hbar$ divided by the interelectronic spacing at the metal-insulator transition. Rather than this fixed spacing, scaling theories of localization[4-6] have proposed that a variable length ξ is the only pertinent scale near the transition. As the density n decreases to the critical value n_c, ξ diverges and reduces the zero-T conductivity $\sigma(0)$ continuously to zero. For a true critical point at n_c, the localization length in the insulator ξ_L has the same critical exponent as ξ.

We have investigated $\sigma(0)$ by measuring the low-electric-field (Ohmic) conductivity of uncompensated Si:P at a series of donor densities and at temperatures down to 1 mK. We have compared our results with the above two descriptions of the transition. The n dependence of $\sigma(0)$ is so sharp that we cannot rule out a discontinuity at Mott's estimated σ_{min}, if there is rounding by ~1% density inhomogeneities. Alternatively we can fit the rise in $\sigma(0)$ above σ_{min} (i.e., for $n/n_c - 1 > 3\%$) by a critical form consistent with a continuous transition. In this region, where we believe inhomogeneities to be unimportant, we find a symmetry between the density dependence of $\sigma(0)$ and that of the dielectric susceptibility in the insulating state,[7] indicating that these quantities can be described by divergent lengths with the same exponent.

Previous experiments on doped semiconductors have been consistent[1] with a σ_{min}, but they have used neither very low T nor closely spaced sample densities. The extensive early work of Fritzsche[8] presents conductivity as a function of donor density for Ge:Sb and Ge:Ga for T down to 2.5 K. Allen and Adkins[9] measured samples of compensated germanium down to 200 mK, or $k_B T/E_I \sim 10^{-3}$, where E_I is the isolated impurity ionization energy. In comparison, our measurements on Si:P utilize $k_B T/E_I \sim 2\times10^{-6}$, but our results at higher T are consistent with previous work. Yamanouchi, Mizuguchi, and Sasaki[10] have also investigated Si:P at low T, but with emphasis on samples which had a high density of surface dislocations.[11,12]

We have made four-probe resistance measurements as a function of T using a lock-in technique and frequencies low enough (~10 Hz) for frequency independence and phase coherence of voltage and current. Wires of Au:Sn were spot welded to a freshly etched sample surface to make contacts whose resistances were less than 10^{-5} the input impedance of the lock-in amplifier and at worst of the order of the sample resistance at any T. The contacts were arranged linearly with an average length between voltage probes of 1 mm along an average cross-sectional area of 0.8×0.5 mm^2. Resistance measurements with movable probes indicated homogeneity in n over a length scale of the order of this sample size. Current flow homogeneity was tested by unnesting the voltage and current leads and observing the noise-limited check voltages $< 10^{-3}$ of the nested voltage.[13] Temperatures down to 1 mK were reached[14] with use of a dilution refrigerator and adiabatic demagnetization of $PrNi_5$. The samples were thermally attached to a copper cold finger through a thin layer of Apiezon grease. Input power was confined to $< 10^{-15}$ W for all samples, and neither heating of the Si crystal lattice nor thermal hysteresis was observed. Crystals of Si:P were obtained from commercial quality Czolchralski growth procedures. The far-infrared absorption of these samples can be described by

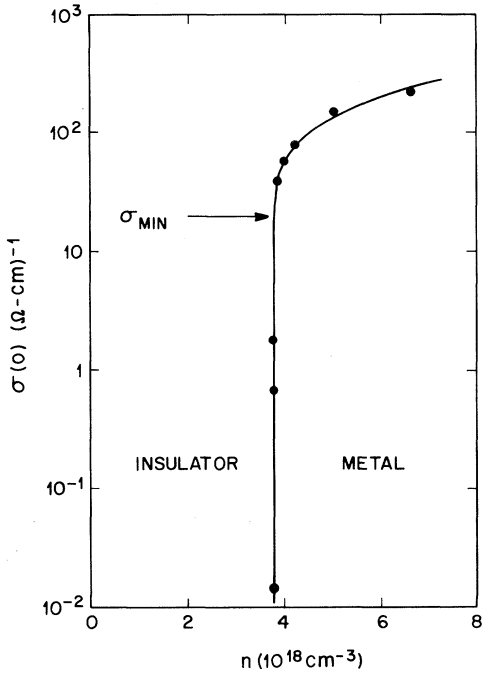

FIG. 1. Semilog plot of zero-temperature conductivity $\sigma(0)$ vs donor density n for metallic samples of Si:P. The transition observed here is extremely sharp, but continuous, with values of $\sigma(0)$ as small as 10^{-3} of σ_{min}. The solid line is a fit by Eq. (2) above σ_{min}.

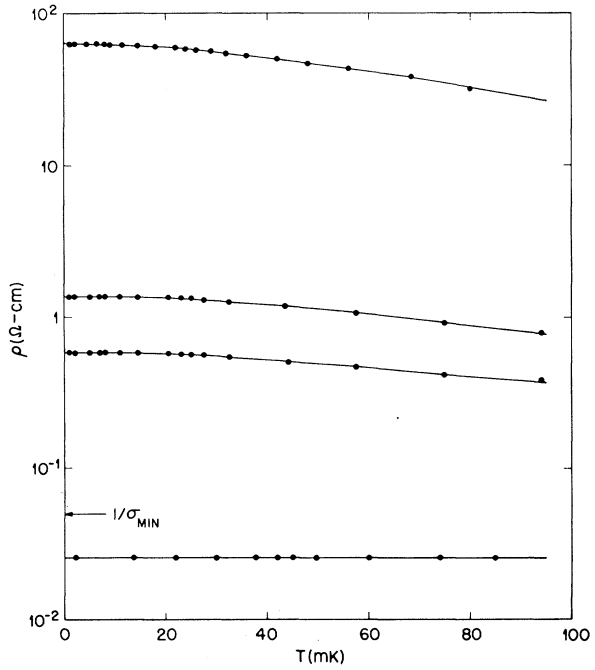

FIG. 2. Graph of the temperature dependence for $1 \leq T \leq 100$ mK of the resistivity ρ of three samples above and one below $1/\sigma_{min}$, emphasizing their metallic nature.

assuming ideal randomness on a microscopic scale.[15]

Figure 1 summarizes our results for $\sigma(0)$ as a function of P donor density n, showing that, near n_c, $\sigma(0)$ changes by over 10^3 when n is varied by less than 1%. We estimate absolute values of n and n_c to be accurate to about 5% (from neutron activation[16]) and relative values to less than 1% (from resistance ratios[12]). Included in the precipitous drop in Fig. 1 are three samples with very small values of $\sigma(0)$. The temperature independence of $\sigma(T)$ as $T \to 0$ K for these samples indicates that they are metallic[1] as shown in Fig. 2 for $T < 100$ mK. In all cases $\sigma(0)$ can be determined accurately by extrapolation as $T \to 0$ K.

According to Mott,[1] the value of σ_{min} is given by

$$\sigma_{min} = C_{min} e^2/\hbar n_c^{-1/3}, \quad (1)$$

where he estimates $C_{min} \sim \frac{1}{20}$ (within a factor of 2) for doped semiconductors. For Si:P, $n_c^{-1/3} = 64$ Å, giving $\sigma_{min} = 20\ (\Omega\ \text{cm})^{-1}$, as indicated in Figs. 1 and 2. Mott has argued[1,17] that it is unlikely that metallic channels of cross section greater than ξ will extend the entire length of macroscopic samples such as ours and produce artificial values of $\sigma(0) < \sigma_{min}$, although we cannot rule out such channels. An estimate of the size of density inhomogeneities that may broaden a possible discontinuity at σ_{min} is the extent of a tail in $\sigma(0)$ below σ_{min}. The sharpness of the rise in $\sigma(0)$ restricts such a tail to $n/n_c - 1 \lesssim 1\%$, or about the same size as our relative uncertainty in determining n. Because of this uncertainty we cannot rule out a jump in $\sigma(0)$ at σ_{min}. We can establish, however, that the density variations which possibly smooth out the transition occur on a scale < 1 mm. Contactless and movable probe measurements at room T show an insignificant variation in n of $\sim 0.04\%$ on this macroscopic scale.

For $n/n_c - 1 > 3\%$, we believe that the effects of inhomogeneities are negligible and we can determine n accurately enough to analyze the data quantitatively. As shown by the solid circles and the curves in Figs. 1 and 3, we can fit the data with the form

$$\sigma(0) = \sigma_c[(n/n_c) - 1]^{\zeta}, \quad (2)$$

with $\sigma_c = 260 \pm 20\ (\Omega\ \text{cm})^{-1}$ and $\zeta = 0.55 \pm 0.1$. Our choice of the form of Eq. (2) is motivated by the result of the scaling theory of localization,[3-6]

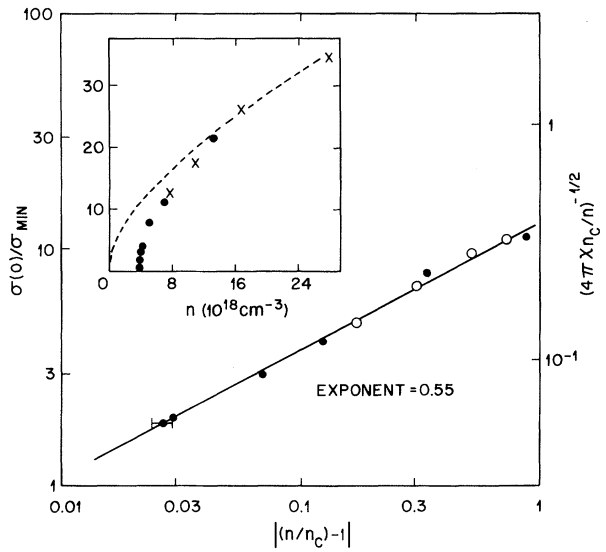

FIG. 3. Log-log plot of $\sigma(0)/\sigma_{min}$ (solid circles, left scale) and the dielectric susceptibility $4\pi\chi$ in normalized form $(4\pi\chi n_c/n)^{-1/2}$ from Ref. 7 (open circles, right scale) vs $|n/n_c - 1|$. The solid line determines the exponent $\nu = 0.55 \pm 0.05$. In the inset, the deviation from a simple screening calculation (Ref. 21) appropriate for $n \gg n_c$ is shown on linear axes in comparison with our values of $\sigma(0)$ (solid circles) and some from Ref. 10 (crosses).

which can be written

$$\sigma(0) = C_L e^2/\hbar\xi , \tag{3}$$

where C_L is a constant and the scale length near n_c has the critical form

$$\xi = \xi_0[(n/n_c) - 1]^{-\nu} . \tag{4}$$

Models of metal inclusions in a dielectric medium[18] as well as classical band and site percolation theories also give the form of Eq. (2) but with $\zeta \approx 1.6$, inconsistent with our results. Non-power law forms, proposed[17] for quantum localization,[20] also do not fit our data.

We have tried to evaluate empirically the region in which precursive behavior becomes important by comparing our results with a theoretical calculation of normal metallic behavior. This calculation of the zero-T conductivity σ_B considers a Fermi gas of electrons distributed in the six conduction band valleys and scattered by the ionized impurities. The calculation excludes intervalley and multiple scattering, and is done with use of the Born approximation and Thomas-Fermi screening, under the assumption, because of the large mass anisotropy, that each electron is effectively screened by electrons in only two valleys—its own and the coaxial valley. The calculation,[21] illustrated by the dashed line in Fig. 3, is expected to be valid for $n \gg n_c$, but below where intervalley and multiple scattering become important, to a level ~20–30%.

The deviation of the data from the dashed curve in Fig. 3 is large for $n/n_c - 1 < 1$, yielding a precursive region where $\xi > \xi_0$. We have used this region, shown in the main part of Fig. 3, for fitting with Eq. (2) and for evaluating the parameters in Eqs. (3) and (4). Current analyses[4-6] of the scaling theory give $\nu \lesssim 1$, and a conductivity scale $\sigma_c \approx \sigma_{min}$. In contrast, we find $\nu = \zeta = 0.55$, and $\sigma_c = 13\sigma_{min} \sim 0.6e^2/\hbar n_c^{1/3}$.

Our fit to $\sigma(0)$ indicates a symmetry of the exponent in the metal with that observed previously[7] in the dielectric susceptibility χ in the insulator. Within the scaling approach,[6,7] $\chi \propto n\xi_L^2$ and so the divergence of ξ_L below n_c should be measured by $(\chi/n)^{1/2}$. We have plotted some of the results for χ as the open circles in Fig. 3 to illustrate that the same exponent describes both ξ above n_c and ξ_L below. For both data sets, n_c was fitted by 3.74×10^{18} cm^{-3}, with absolute uncertainty $\pm 0.2\times10^{18}$ cm^{-3}.

The current localization models of scaling restrict their region of applicability to $\sigma(0) \lesssim \sigma_{min}$ or $n/n_c - 1 < 1\%$, where our limits on density accuracy and homogeneity do not rule them out. Within this same narrow density region Mott's σ_{min} remains possibly a true minimum, although we measure metallic $\sigma(0)$ values down to $10^{-3}\sigma_{min}$. However, the observed symmetry of the divergent lengths and the measured characteristic conductivity support a general scaling description of the precursive behavior for $n/n_c - 1 \lesssim 1$ near the metal-insulator transition in a random, three-dimensional system.

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Four-Particle Radiative Transitions of Biexcitons and Multiple Bound Excitons in Si

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In this paper the observation of sharp and very weak emission lines in phosphorous-doped silicon near twice the band-gap energy is reported. The line with the highest energy can be attributed to the total radiative annihilation of a free biexciton. The other three lines originate from the decay of two electron-hole pairs in a multiple bound exciton complex of two, three, and four excitons.

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In recent years there has been a large number of publications dealing with series of sharp excitonic emission lines connected with shallow impurities in the semiconductors with indirect band structure Si,[1] Ge,[2] SiC,[3] and GaP[4] at low temperatures. Originally the lines have been attributed to the radiative decay of multiple bound excitons (MBE). A more detailed model, called the "shell model," has been proposed by Kirczenow[5] and supported experimentally mainly by Thewalt.[1] After considerable controversy it is now generally accepted that the shell model adequately describes most of the experimental properties of the MBE's.[6] Nevertheless, no direct proof of the many-particle nature has been given so far. As a direct proof, in this paper the observation of emission lines at about twice the band-gap energy is reported for the first time. They are ascribed to the simultaneous decay of two excitons bound in a multiple exciton complex.

Some years ago, Betzler, Weller, and Conradt observed a green emission from highly excited silicon at room and liquid-nitrogen[7] as well as at liquid-helium temperatures.[8] The broad emission band which appears at low temperature was explained by the simultaneous radiative recombination of two electrons and two holes within the electron-hole droplets (EHD).

If MBE's really exist, analogous transitions should lead to sharp emission lines near $2E_g$. In order to estimate the expected luminescence intensity, one can compare the transition probabil-

