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Metal-insulator transition in Si:As

P. F. Newman and D. F. Holcomb
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853
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Electrical conductivity σ of uncompensated Si:As has been measured in the temperature range 1.8—300 K, for a range of values of arsenic concentration $n_{\rm As}$ from 7.4×10^{18} to 10.5×10^{18} cm^{-3}. The value of n_c, the critical concentration for the metal-insulator transition, is $(7.8^{+0.3}_{-0.5})\times10^{18}$ cm^{-3} for Si:As. The ratio of n_c for Si:As to n_c for Si:P is about 20% higher than that given by a simple argument based on the difference in effective Bohr radii.

Interest in the study of the transition from the semiconducting to metallic state in doped semiconductors has been recently renewed by the work of Rosenbaum *et al.*[1,2] They have shown that an examination of the electrical conductivity at very low temperatures yields new insight into the nature of the metal-insulator (*M-I*) transition in disordered systems.

We report measurements of the low-temperature electrical conductivity in a companion system, Si:As, as a function of temperature at various donor concentrations. The primary purpose of these measurements is to compare the results with the prototype system Si:P. This comparison permits tests of the generality of relevant models.

In Mott's original model,[3] the *M-I* transition for an impurity system such as Si:P or Si:As should occur at a value of n_D, the donor concentration, given by the relationship

$$(n_D)_{\rm crit}\equiv n_c=(0.25a_{\rm H}^*)^{-3}\ , \qquad (1)$$

where $a_{\rm H}^*$ is an effective Bohr radius. Edwards and Sienko[4] have recently collected data on a wide variety of systems and have shown the remarkable extent to which this simple picture based on screening describes *M-I* transitions. Our value of n_c for Si:As, when combined with that of Rosenbaum *et al.* for Si:P, gives a ratio $(n_c)_{\rm As}/(n_c)_{\rm P}=2.09\pm0.12$, whereas the ratio given by Eq. (1) is 1.64 if one uses donor ionization energy as a measure of $a_{\rm H}^*$.

Recent interest in the semiconductor systems has also focused on the temperature and concentration dependence of the electrical transport properties for samples with concentrations near n_c. The work of Rosenbaum *et al.* on Si:P and a recent paper by Thomas *et al.*[5] which deals with Ge:Sb make extensive reference to relevant features of the current theoretical models.[6,7] We restrict ourselves to characterizing the experimental results on Si:As, and to a comparison with Si:P and *n*-type germanium.

Our experimental samples were cut from the centers of wafers 380 μ thick that were sliced from a Czochralski-grown boule of 5 cm diameter. We made a resistivity map of the center of each wafer, then cut samples whose dimensions were 4 mm long by 1.1 mm wide by 0.4 mm thick. Four leads of Au:2%Sn alloy wire were attached to each freshly etched sample with a technique developed by Capik[8] and used by Rosenbaum *et al.* Contact resistance was typically 0.4 Ω at room temperature and decreased at lower temperatures. We estimate that a typical inhomogeneity of arsenic concentration over the region of the sample sensed by the voltage leads was 0.3%.

Samples were mounted on a sapphire substrate which was in turn mounted on a copper block whose temperature was controlled between 1.8 and 200 K. The temperatures reported are based on a calibration of our working carbon-glass thermometer against a second carbon-glass unit calibrated by Lakeshore Cryotronics. We estimate the uncertainty in *relative* measurements of temperature in any given run to be about ±0.02 K near 4.2 K.

We used dc measurement techniques throughout. All voltages were measured using a Keithley model 181 nanovoltmeter. Currents used ranged from 10 μA to 10 mA. At 10 mA current at 1.8 K, any resistance change due to heating effects was less than 1%. A measuring current of 100 μA was used for most measurements. On the basis of the investigations of Rosenbaum, Andres, and Thomas[9] we are convinced that the conductivity values we report have not been influenced by resistive heating.

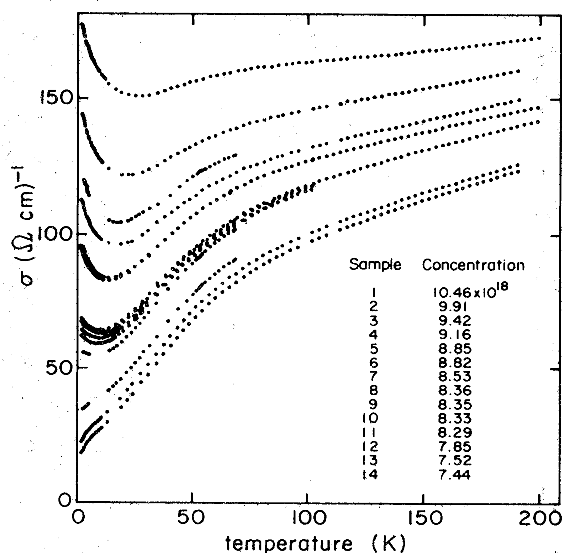

FIG. 1. Conductivity of samples of Si:As vs absolute temperature. The key lists the samples in the same vertical order as their conductivity curves appear in the figure. The corresponding arsenic concentrations are indicated.

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In order for our results to be most useful, we need precise determination of both relative and absolute values of n_{As}. In doped semiconductors, the property which can be most conveniently used as a measure of impurity concentration is the room-temperature resistivity. Unfortunately, it does not yield a direct measure of n_D, and a calibration scale based on some absolute measurement is also needed. For Si:P, Mousty *et al.*[10] compared measurements of resistivity at 296 K with absolute determination by neutron activation analysis of n_P, the phosphorus concentration. The values of n_P used by Rosenbaum *et al.* were derived from the Mousty scale. For Si:As, we find no study in the literature comparable to that of Mousty *et al.* for Si:P. Recent studies[11] suggest that over the concentration range of interest here, arsenic concentrations will be slightly underestimated by the use of the phosphorus calibration curve, but by no more than 10%. We use the room-temperature resistivity calibration curve recently established for Si:P by Thurber *et al.*[12] on the basis of a merging of the data of Mousty *et al.* with some of their own measurements. (See *Note added in proof.*)

Our experimental results are shown in Fig. 1, in a linear plot of electrical conductivity as a function of temperature, $\sigma(T)$. For samples with $n_{As} > 8.2\times10^{18}$ cm^{-3}, the conductivity falls as T increases from 1.8 K, reaches a minimum, and then rises. Note that the conductivity minimum shifts to higher temperature as n_{As} increases. For samples with $n_{As} < 8.2\times10^{18}$ cm^{-3}, there is no minimum and σ is still falling at our lowest temperature, 1.8 K. Rosenbaum *et al.*[2] observed similar behavior in Si:P.

We use the analysis procedure of Rosenbaum *et al.* to obtain the value of n_c from our data. A value of $\sigma(0)$ for each sample is determined by extrapolating each of the curves of Fig. 1 to $T=0$ K. In making this extrapolation, we fit the data below 4 K with the equation $\sigma(T)=\sigma(0)+mT^{1/2}$. We note that there is theoretical justification for the use of this function.[5] The curve fitting yields values of $\sigma(0)$ and m. From the curve fitting, we find that values of m for samples with $n_{As} > 8.8\times10^{18}$ cm^{-3} fall in the range from -7 to -11 Ω^{-1}cm^{-1}K$^{-1/2}$, in good agreement with Rosenbaum *et al.*[2] For samples at lower concentration, we judge that the temperature range of our measurements is not adequate to yield reliable values of m.

We plot our values of $\sigma(0)$ as a function of n_{As} in Fig. 2. Shown at the top of Fig. 2 is the scale of measured values of $\rho_{296\,K}$ from which the values of n_{As} were obtained. The solid line is a best fit of the values of $\sigma(0)$ in the concentration range with $n_{As} > 8.2\times10^{18}$ cm^{-3}. The measurements of Rosenbaum *et al.* on Si:P make it clear that for samples very near the *M-I* transition, one must make measurements in the millikelvin temperature range in order to extract reliable values of $\sigma(0)$. On the other hand, for samples with concentrations such that $\sigma > 2\sigma_{min}$, where σ_{min} is Mott's minimum metallic conductivity, one can reliably extrapolate from conductivity values at 2 K to obtain $\sigma(0)$.[13] This guideline leads to the exclusion from our fit of samples with $n_{As} < 8.2\times10^{18}$ cm^{-3}. The fitting procedure assumes a functional form, $\sigma(0)=\sigma_0(n/n_c-1)^\nu$, with three fitting parameters: σ_0, ν, and n_c. The fit yields $\sigma_0=381$ Ω^{-1}cm$^{-1}=16\sigma_{min}$,[14] $\nu=0.64^{+0.20}_{-0.15}$, and $n_c=(7.8^{+0.3}_{-0.5})\times10^{18}$ cm^{-3}. For Si:P,

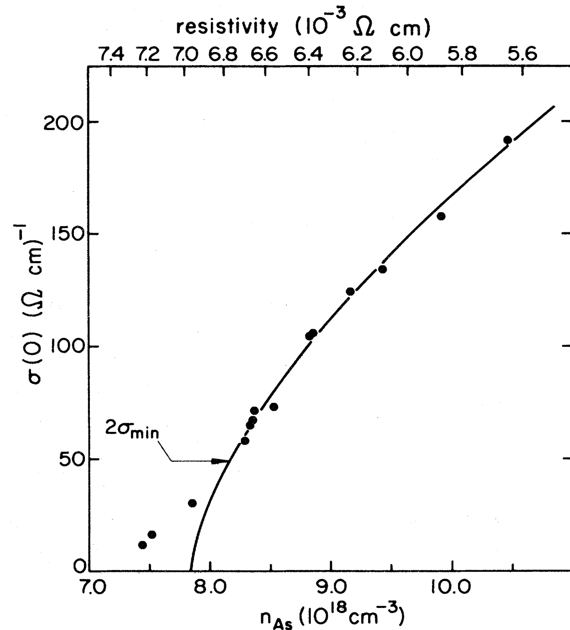

FIG. 2. Extrapolated $T=0$ conductivity $\sigma(0)$ vs arsenic concentration n_{As}. The scale of measured values of $\rho_{296\,K}$, from which values of n_{As} are derived, is also given at the top. The solid line is the best fit for the function $\sigma=\sigma_0(n/n_c-1)^\nu$, for data from samples with $n_{As} > 8.2\times10^{18}$; σ_0, n_c, and ν are fitting parameters.

TABLE I. Ratios of n_c values for pairs of donors.

Donor pair	$[(a_H^*)_2/(a_H^*)_1]^3$	$[(n_c)_1/(n_c)_2]_{expt}$	Source
Si:As Si:P	1.64	2.09±0.15 1.83±0.25 2.0	This work and Ref. 1 Ref. 16 Ref. 17
Ge:As Ge:Sb	2.2	3.1	Ref. 18
Ge:P Ge:Sb	1.9	2.4	Ref. 18

Rosenbaum *et al.*[1] found $\nu=0.55\pm0.1$. The value of n_c corresponds to a resistivity of $\rho_c=6.97\times10^{-3}$ Ω cm at 296 K. The uncertainty in n_c is associated with the analysis procedure which leads to Fig. 2. We have not included any estimate of uncertainties associated with use of the Si:P resistivity scale for Si:As. The error in $\rho_{296\,\mathrm{K}}$ is only 0.5%.

A primary goal in our determination of n_c for Si:As is to observe how n_c varies with different donors in a common host material. Table I displays our experimental value of $(n_c)_{\mathrm{As}}/(n_c)_{\mathrm{P}}$ derived from the combination of our value of n_c for Si:As with that determined by Rosenbaum *et al.* for Si:P, $(3.74\pm0.2)\times10^{18}$ cm^{-3}. Also given are some results drawn from previous investigations. It also shows the result calculated from Eq. (1). The experimental value of $(a_{\mathrm{H}}^*)_1/(a_{\mathrm{H}}^*)_2$ is taken to be $(E_D)_2/(E_D)_1$, where E_D is the measured donor ionization energy. Values of E_D are 53.5 meV for Si:As and 45.3 meV for Si:P.[15] The value of the n_c ratio for Si:As and Si:P derived from the work of Castner *et al.*[16] depends on dielectric measurements in samples with $n_D < n_c$. We have obtained a third value of the ratio from the ESR work of Pifer[17] by matching patterns of concentration and temperature dependence of ESR linewidth in the two materials.

The germanium data in Table I is extracted from electrical conductivity measurements of Fritzsche.[18] His samples were located at widely spaced values of n_D. We determined the values given in the table by interpolation from the Fritzsche data. Thus the uncertainty in the ratios is fairly large, and cannot be determined quantitatively. Values of E_D for the germanium systems are 12.7 meV for Ge:As, 9.7 meV for Ge:Sb, and 12.0 meV for Ge:P.[19]

Our experimental value of the ratio $(n_c)_{\mathrm{As}}/(n_c)_{\mathrm{P}}$ is about 20% higher than the prediction of Eq. (1). Our analysis of Fritzsche's data in germanium suggests that corresponding experimental ratios also depart measurably from the Mott model. Thus while the simple Bohr-radius argument gives a rough measure of the scaling of n_c, it seems clear that a more detailed picture of wave-function overlap is required in order to quantitatively describe the effects of the different central-cell potentials for different impurities. The other possibility, of course, is that effects of disorder, which are outside the original Mott model, change the ratio from the simple scaling with $(a_{\mathrm{H}}^*)^{-3}$.

We have fixed our attention on ratios of values of n_c. It is important to note that slightly different calibration curves have been used by different investigators in converting values of $\rho_{296\,\mathrm{K}}$ to values of n_D. Consequently, absolute values of n_c from different investigators[16,17] may not be directly comparable to ours.

Note added in proof. In the time interval since submission of this paper, we have completed a neutron activation determination of arsenic concentrations. These results increase all values of n_{As} given in Figs. 1 and 2 by 9%. Consequently, the value of n_c for Si:As is 8.5×10^{18} cm^{-3} rather than the quoted value of 7.8×10^{18} cm^{-3}, which was based on the Si:P room-temperature resistivity calibration scale. This new value places the ratio of n_c for Si:As to n_c for Si:P at a value about 40% higher than the ratio predicted by Eq. (1). All three values of the ratio given in the third column of Table I for the pair Si:As and Si:P also increase by 9%, since the values drawn from Refs. 16 and 17 also depended upon applying the Si:P resistivity calibration scale to Si:As.

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[14] They calculate a value of 20 Ω^{-1}cm^{-1} for $\sigma_{\min}$ in Si:P. For values of $\sigma_{\min}$ in doped semiconductors, this is a natural quantity to use to scale a_{H}^*. Since a_{H}^* is about 20% smaller for Si:As than for Si:P, we use the value 24 Ω^{-1}cm^{-1} for $\sigma_{\min}$ in Si:As. Thus for Si:As, $\sigma_0=16\sigma_{\min}$. For Si:P, Rosenbaum *et al.* found a similar result, $\sigma_0=13\sigma_{\min}$.

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