Comment on "Critical behavior of the zero-temperature conductivity in compensated silicon, Si:(P,B)"

A. Möbius
Zentralinstitut für Festkörperphysik und Werkstofforschung der Akademie der Wissenschaften der Deutschen Demokratischen Republik, DDR-8027 Dresden, German Democratic Republic
(Received 24 October 1988)

In a recently published conductivity study of Si:(P,B) very close to the metal-insulator transition, Hirsch and co-workers performed the zero-temperature extrapolation by using the relation $\sigma(T)=\sigma(0)+mT^{1/2}+BT^{3/4}$, based on modern localization theory. This extrapolation is critically reconsidered studying the temperature dependence of the logarithmic derivative, $d\ln\sigma/d\ln T$.

The metal-semiconductor transition (MST) in disordered three-dimensional systems has been a matter of intensive debate for more than ten years. Nowadays, the experiments are mainly interpreted in terms of a continuous transition at $T=0$.[1] However, the final decision concerning the character of the transition has been a very difficult one due to the zero-temperature extrapolation included in most of the experimental studies. In particular, near the transition it is even difficult to decide reliably whether a certain sample is metallic or semiconducting. These two points are also inherent in the investigation of the conductivity of compensated silicon, Si:(P,B), near the MST by Hirsch and co-workers.[2] These authors analyze their obviously very careful measurements in terms of the ansatz

$$\sigma(T)=\sigma(0)+mT^{1/2}+BT^{3/4}\ , \qquad (1)$$

based on modern localization theory. They classify the samples as metallic as long as the zero-temperature extrapolation, $\sigma(0)$, is positive. This zero-temperature extrapolation and the classification related are reanalyzed in the present Comment.

Consider the logarithmic derivative $w(T)=d\ln\sigma/d\ln T$, which is far more sensitive than the conductivity itself. Equation (1) implies that $w(T)$ vanishes as $T\rightarrow 0$ according to

$$w(T)=(0.5mT^{1/2}+0.75BT^{3/4})/\sigma(T)\ , \qquad (2)$$

for the metallic samples. This conclusion has been checked in the following way. Figure 1 of Ref. 2 contains $\sigma(T)$ points for five samples, which are labeled A-63, B-265, B-270, B-285, and B-310 in the original paper by Hirsch and co-workers. These data were digitized using an image-processing system. All combinations of k neighboring points, $k=6$, were analyzed by means of linear regression considering $\ln\sigma$ as a function of $\ln T$. The T value corresponding to the slope obtained was approximated by the geometrical average, $\{\prod_{i=1}^{k}T_i\}^{1/k}$. This procedure ensures that stochastic and numerical errors are kept sufficiently small. The results are shown in Fig. 1. For comparison, fits according to ansatz (1) were performed. The $\sigma(0)$ values obtained from these $\sigma(T)$ fits, 5.8, 14.5, 30.4, and 50.2 $\Omega^{-1}\,\text{cm}^{-1}$ for samples B-265, B-285, B-310, and A-63, respectively, agree well with the data given by Hirsch *et al.* 6.1, 15.4, 31.3, and 50.1 $\Omega^{-1}\text{cm}^{-1}$.[2] The corresponding $w(T)$ relations are included as solid lines in Fig. 1.

Figure 1 shows good agreement between $w(T)$ values, obtained directly from experimental data, and fit curves. However, there is no experimental evidence that $w(T)\rightarrow 0$ as $T\rightarrow 0$ for samples B-265 and B-285, classified as metallic in Ref. 2. The experimental $w(T)$ values related do not significantly vary within the

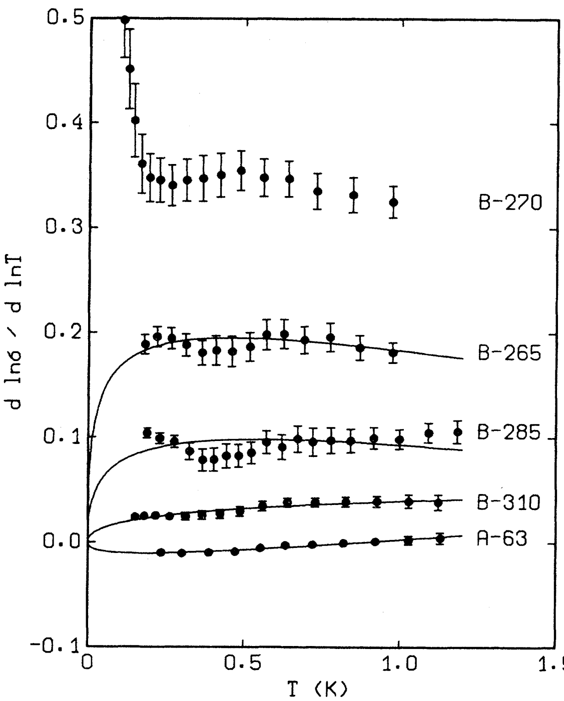

FIG. 1. Logarithmic derivative $w(T)=d\ln\sigma/d\ln T$ vs T. The error bars, given only if they exceed the symbol size, denote the 3σ bounds related to the stochastic errors arising in the digitization procedure. For comparison, fits according to Eq. (1) are included as solid lines. The samples are labeled according to the original paper (Ref. 2).

measuring temperature interval, and the fit curves exhibit broad plateaus in this region. Both fit curves change their character qualitatively at about 0.2 K. A steep decrease, which has no precursor in the measuring interval, occurs below this temperature. If $w(T \rightarrow 0)$ would alternatively tend to a finite positive value, as it seems to be suggested by Fig. 1, or to infinity, as for the semiconducting sample B-270, $\sigma(T \rightarrow 0)$ would vanish and only activated conduction would be present. Hence, the extrapolation according to Eqs. (1) and (2) has to be regarded as uncertain, even the character of conduction remains open. Measurements down to about 30 mK, as performed for sample B-270 in Ref. 2, should be sufficient to check whether $w(T)$ would significantly tend to zero according to Fig. 1.

Furthermore, it should be noted that, for sample B-310, $w(T)$ remains approximately constant below about 0.5 K. The above discussion might apply as well here. However, in this case, and in the case of the clearly metallic sample A-63, the values of $|w(T)|$ are too small to draw reliable conclusions.

The consideration above agrees with the critical remarks by Hirsch *et al.* concerning the reliability of $\sigma(0)$ values below 10 $\Omega^{-1}\text{cm}^{-1}$. These authors point to the similarity between the samples B-270 and B-265, which they regarded as semiconducting and metallic, respectively. Furthermore, samples B-285 and B-310, classified as metallic by them, do not qualitatively differ from the sample B-265 according to Fig. 1. This behavior might alternatively be interpreted in terms of a phenomenological model of $\sigma(T,n)$ close to the MST, developed for amorphous $Si_{1-x}Cr_x$ in Ref. 3, and shown also to be applicable to other substances in Ref. 4. Based on "generalized symmetries" within $\sigma(T,n)$, that analysis avoids $T \rightarrow 0$ extrapolations for individual samples. According to Refs. 3 and 4, samples B-265, B-285, and B-310 should be semiconducting. Moreover, below about 0.5 K, $w = d\ln\sigma/d\ln T$ should increase as T is diminished, where $|dw/dT|$ should vanish as $w \rightarrow 0$. In order to get more insight into this complicated problem, it would be very interesting to check these predictions by reanalyzing the complete experimental data set of Ref. 2 and by an additional extension of the measurements to temperatures below 100 mK.

I am indebted to E. Müller and H. Wendrock for digitizing the data from Fig. 1 of Ref. 2. Critical discussions with H. Eschrig, M. Richter, and R. Richter are gratefully acknowledged.

[1]R. F. Milligan, T. F. Rosenbaum, R. N. Bhatt, and G. A. Thomas, in *Electron-Electron Interactions in Disordered Systems,* edited by A. L. Efros and M. Pollak (North-Holland, Amsterdam, 1985), p. 231.

[2]M. J. Hirsch, U. Thomanschefsky, and D. F. Holcomb, Phys. Rev. B **37**, 8257 (1988).

[3]A. Möbius, D. Elefant, A. Heinrich, R. Müller, J. Schumann, H. Vinzelberg, and G. Zies, J. Phys. C **16**, 6491 (1983); A. Möbius, H. Vinzelberg, C. Gladun, A. Heinrich, D. Elefant, J. Schumann, and G. Zies, *ibid.* **18**, 3337 (1985).

[4]A. Möbius, J. Phys. C **18**, 4639 (1985).