Critical behavior of the conductivity of Si:P at the metal-insulator transition under uniaxial stress

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We report new measurements of the electrical conductivity $\sigma$ of the canonical three-dimensional metal-insulator system Si:P under uniaxial stress $S$. The zero-temperature extrapolation of $\sigma(S, T \to 0) \sim |S - S_c|^\mu$ shows an unprecedently sharp onset of finite conductivity at $S_c$ with an exponent $\mu = 1$. The value of $\mu$ differs significantly from that of earlier stress-tuning results. Our data show dynamical $\sigma(S, T)$ scaling on both metallic and insulating sides, viz. $\sigma(S, T) = \sigma_c(T) \cdot F(|S - S_c| /T^\nu)$ where $\sigma_c(T)$ is the conductivity at the critical stress $S_c$. We find $y = 1/2\nu = 0.34$ where $\nu$ is the correlation-length exponent and $z$ the dynamic critical exponent.

Quantum phase transitions have become of steadily increasing interest in recent years [1]. These continuous transitions ideally occur at temperature $T = 0$ where quantum fluctuations play the role corresponding to thermal fluctuations in classical phase transitions. In particular, certain types of metal-insulator transitions (MIT) such as localization transitions have been studied extensively. Experimentally, the MIT may be driven by an external parameter $t$ such as carrier concentration $N$, uniaxial stress $S$, or electric or magnetic fields. Generally, electron localization might arise from disorder (Anderson transition) or from electron-electron (e-e) interactions (Mott-Hubbard transition) [2]. In Nature, these two features go hand in hand. For instance, the disorder-induced MIT occurring as a function of doping in threedimensional ($d = 3$) semiconductors where the disorder stems from the statistical distribution of dopant atoms in the crystalline host, bears signatures of e-e interactions as evidenced from the transport properties in both metallic [2] and insulating regimes [4]. This makes a theoretical treatment of the critical behavior of a MIT exceedingly difficult. Even for purely disorder-induced transitions, the critical behavior of the zero-temperature dc conductivity, $\sigma(0) \sim |t - t_c|^\nu$ where $t_c$ is the critical value of $t$, is not well understood. Theoretically, $\mu$ is usually inferred from the correlation-length critical exponent $\nu$ via Wegner scaling $\mu = \nu(d-2)$. Numerical values of $\nu$ range between 1.3 and 1.6 [5,6].

Experimenterly, it has long been suggested that the critical behavior of the conductivity falls into two classes: $\mu \approx 0.5$ for uncompensated semiconductors and $\mu \approx 1$ for compensated semiconductors and amorphous metals [5]. However, there appears to be no clear physical distinction between these materials that would justify different universality classes. While many different materials were reported to show $\mu \approx 1$, the exponent $\mu \approx 0.5$ was largely based on the very elegant experiments by Paalanen and coworkers [6,7], where uniaxial stress was used to drive an initially insulating uncompensated Si:P sample metallic. This allows to fine-tune the MIT since the stress can be changed continuously at low $T$ thus eliminating geometry errors incurred when different samples are employed in concentration tuning the MIT.

As always when dealing with critical phenomena, the range of critical behavior is a source of controversy. A few years ago we suggested [1] to limit the critical concentration region in doped semiconductors on the metallic side of the MIT to samples where $\sigma(T)$ actually decreases with decreasing $T$, i.e. the sample becomes less conducting when approaching the MIT. In doped semiconductors, $\sigma(T)$ is nearly independent of $T$ at the crossover concentration $N_{cr}$, with a value $\sigma_{cr}$ of a few times $10 \Omega^{-1} \text{cm}^{-1}$, e.g. $\sigma_{cr} \approx 40 \Omega^{-1} \text{cm}^{-1}$ in Si:P. $\sigma(T)$ exhibits a negative temperature coefficient above $N_{cr}$ which is explained in terms of e-e interactions [8]. Typically the critical region $N_c < N < N_{cr}$ is within 10% or less of the critical concentration $N_c$. This eliminates a large number of studies purporting to show $\mu = 0.5$ where actually only a few samples in the critical regime were investigated. Even the recent study on transmutation-doped Ge:Ga where $\mu = 0.5$ was suggested, presents only three metallic samples in the critical region below $\sigma_{cr} \approx 10 \Omega^{-1} \text{cm}^{-1}$ [9].

An earlier study of a large number of Si:P samples showed that the conductivity exponent $\mu$ changed from $\mu = 0.64$ for $N > N_{cr} \approx 1.1 N_c$ to 1.3 for $N_c < N < N_{cr}$ [7]. On the other hand, sample inhomogeneities might affect the behavior very close to $N_c$. For this reason, data for stress-tuning with stress close to the critical value were discarded in the earlier study, leading to $\mu = 0.5$ [6,7]. It is therefore absolutely necessary to perform additional stress-tuning experiments on Si:P with finely tuned stress values including data on the insulating side to check for the critical behavior.

The notion of a quantum phase transition allows a second important aspect to be addressed, namely the interdependence of static and dynamic behavior. The dy-
namics is reflected in the finite-temperature behavior of critical quantities. Concerning the MIT in heavily-doped semiconductors, this point has not received much attention from the experimental side. A first attempt was made using the scaling function

$$\sigma(t, T) = (t - t_c)^\nu F(T/(t - t_c)^{z\nu})$$

(1)

where $z$ is the dynamic critical exponent. This relation is often referred to as dynamic scaling. Approximate dynamic scaling was observed for Si:P on the metallic side of the MIT with $t = N$, yielding $\mu = 1.3$ and $z = 2.4$. On the other hand, the stress-tuning data did not obey scaling. Very recently, Bogdanovich et al. demonstrated that conductivity data for Si:B under uniaxial stress obey very nicely the dynamic scaling on both metallic and insulating sides, yielding $\mu = 1.6$ and $z = 2$, while concentration tuning of $\sigma(0)$ on the same system had suggested $\mu = 0.63$. This large difference is not understood at present. In this situation, an examination of possible dynamic scaling of the canonical metal-insulator system Si:P appears of utmost importance in order to resolve the question of critical behavior and to appraise the possibly strongly different roles of stress and concentration in tuning the MIT.

In this paper, we report on stress tuning of the MIT of Si:P by measuring the electrical conductivity down to 15 mK. We find by extrapolating to $T = 0$ an unprecedently sharp onset of $\sigma(t, 0)$ which allows to unambiguously extract $\mu \approx 1$. In addition, dynamic scaling yielding $z \sim 3$ is found. The value of $\mu$ is in reasonable agreement with that derived from concentration tuning. We further demonstrate that stress tuning and concentration tuning lead to very different $T$ dependencies of $\sigma$.

The samples were taken from the same Si:P crystals which have been employed previously. Here we report on investigations on two crystals with $N = 3.21 \cdot 10^{18} \text{cm}^{-3}$, just below the critical concentration $N_c = 3.52 \cdot 10^{18} \text{cm}^{-3}$ as determined for our samples. Similarly grown samples with an even higher concentration ($N \approx 7 \cdot 10^{19} \text{cm}^{-3}$) showed no sign of P clustering as investigated with scanning tunneling microscopy. The samples were cut to a size of $15 \times 0.8 \times 0.9 \text{mm}^3$ and contacted with four Au leads by spark welding, with the voltage leads $\sim 6 \text{mm}$ apart. The sample was mounted in a $^4\text{He}$-activated uniaxial pressure cell equipped with a piezoelectric force sensor. The stress was applied along the [100] direction which was the most elongated dimension of the sample. The stress was determined from the ratio of the area of the cell base plate and the sample cross section. Calibration of the cell showed a linear increase of force with pressure applied at room temperature to gaseous He, with no hysteresis between increasing and decreasing pressure. The cell, incorporating a thermal shield, was tightly screwed to the mixing chamber of a dilution refrigerator. During one run a thermometer was attached to the sample showing that temperature deviations to the main thermometer directly mounted at the mixing chamber were less than 0.5 mK at the lowest measuring temperature of 15 mK. The conductance was measured with a LR 700 resistance bridge at 16 Hz.

Fig. 1 shows the electrical conductivity $\sigma(T)$ of sample 1 ($N = 3.21 \cdot 10^{18} \text{cm}^{-3}$) for uniaxial pressures between 1 and 3.05 kbar. The data are plotted vs. $\sqrt{T}$ which is the $T$ dependence expected due to e-e interactions and indeed observed well above the MIT, $\sigma(T) = \sigma_0 + m\sqrt{T}$ with $m < 0$. The smooth curves are in fact polygons connecting adjacent data points (see Fig. 2a for a set of actual data points). Under uniaxial stress between 1 and 2.57 kbar the $\sigma(T)$ curves evolve smoothly from insulating to metallic behavior with $m > 0$, and $\sigma(T)$ becomes nearly independent of $T$ at a value $\sigma_{cr} \approx 12\Omega \text{cm}^{-1}$ at $\sim 2.7$ kbar. For larger stress $\sigma(T)$ passes over a shallow maximum signaling the crossover to $m < 0$, as observed with concentration tuning. It is interesting to note that $\sigma_{cr}(S) \approx 0.3 \sigma_{cr}(N)$, thus severely limiting the critical region. Our data do not exhibit the precipitous drop of $\sigma(T)$ below $\sim 40 \text{mK}$ for pressures closest to the MIT, in distinction to the earlier stress-tuning work on Si:P extending to $3 \text{mK}$. Instead, our $\sigma(T)$ data exhibit a $T$ dependence that varies only gently with stress.

Closer inspection shows that the data near the MIT
are actually better described by a $T^{1/3}$ dependence for low $T$ as can be seen from Fig. 2a for a few selected pressures in the immediate vicinity of the MIT. $\sigma(0)$ obtained from the $T^{1/3}$ extrapolation to $T = 0$ is shown in Fig. 2b, together with data for sample 2 ($N = 3.43 \cdot 10^{18}$ cm$^{-3}$) (see Fig. 3 for $\sigma(T)$ of this sample for a few representative uniaxial pressures). $\sigma(0)$ is plotted linearly vs. $S$, yielding $S_c = 1.75$ kbar for sample 1 and 1.54 kbar for sample 2. Note that the critical stress $S_c$ is quite well defined, as $\sigma(0)$ breaks away roughly linearly from zero within less than 0.1 kbar. Applying our criterion for the critical region, the analysis should be limited to data with $\sigma < \sigma_c \approx 12 \Omega^{-1} cm^{-1}$. In this range the critical exponent $\mu$ is 0.96 and 1.09 for sample 1 and 2, respectively. $\mu \approx 1$ are found also when the more conventional $\sqrt{T}$ extrapolation is employed as can be inferred from Fig. 1. This behavior contrasts with the earlier stress-tuning data [8] reproduced in the inset of Fig. 2b, where appreciable rounding close to $N_c$ is visible as compared to our samples when plotted against $S - S_c$ (see also [12]). However, those $\sigma(0)$ data between 4 and 16 $\Omega^{-1} cm^{-1}$ are compatible with linear dependence on uniaxial stress.

Fig. 3 shows $\sigma(T)$ of sample 2 for a range of selected uniaxial pressures, again applied along [100]. The overall behavior is very similar to that of sample 1. The fact that $\sigma_c$ is the same for both samples is nevertheless surprising given the difference in $S_c$. It has been suggested that tuning with $S$ or $N$ should yield the same critical exponents $[8–10,19]$. The decrease of $N_c$ with uniaxial stress is attributed to the admixture of the more extended 1s($E$) and 1s($T_2$) excited states to the 1s($A_1$) groundstate of the valley-orbit split sixfold donor 1s multiplet [19]. However, comparison of $\sigma(T)$ for various $S$ and $N$ (Fig. 3) reveals that stress and concentration tuning lead to strikingly different $T$ dependences of the conductivity in the vicinity of the MIT. As the exact origin of the $\sigma(T)$ behavior close to the MIT is unknown, we cannot offer an explanation for the different behavior which, of course, must arise from the change of donor wave functions under uniaxial stress. In this respect, experiments on similar samples for stress applied along different directions leading to different types of mixing among the states of the 1s multiplet will be helpful. The fact that stress was applied to different directions in the previous and present study, i.e. [123] and [100], respectively, may well be one reason for the different behavior of $\sigma(T)$.

We finally turn to the scaling behavior of $\sigma$ at finite temperatures using the data of sample 1. We employ the scaling relation [12].
where $\sigma_c(T) = \sigma(t_c, T)$ is the conductivity at the critical value $t_c$ of the parameter $t$ driving the MIT. This scaling relation is equivalent to Eq. (1), both are derived from the general scaling relation

$$\sigma(t, T) = \sigma_c(T)F\left((t-t_c)/T^\nu\right)$$

where $b$ is a scaling parameter. If the leading term to $\sigma_c(T)$ is proportional to $T^x$, one obtains $x = \mu/\nu z$ and $y = 1/\nu z$ from a scaling plot. Fig. 1 and 2a show that $\sigma$ for $S$ close to $S_c$ does not exhibit a simple power-law $T$ dependence over the whole $T$ range investigated. We therefore determine $\sigma_c(T)$ self-consistently in the following manner. The critical stress for sample 1 is taken from the above analysis as $S_c = 1.75$ kbar. In order to obtain $\sigma_c(T)$, we interpolate linearly between the two $\sigma(T)$ curves for $S = 1.72$ and 1.77 kbar. The resultant $\sigma_c(T)$ is then fitted by the function $\sigma_c(T) = aT^2(1 + dT^w)$ with $a = 6.01\Omega^{-1}\text{cm}^{-1}$, $x = 0.34$, $d = -0.202$, $w = 0.863$, and $T$ is expressed in K. Here the $dT^w$ term presents a correction to the critical dynamics. This $\sigma_c(T)$ curve is shown in a dashed line in Fig. 2a. All $\sigma(S, T)$ curves with $1.00$ kbar $< S < 2.34$ kbar up to 800 mK are then used for the scaling analysis according to Eq. (2). The same procedure was repeated for other choices of $\sigma_c(T)$ between the two measured $\sigma(T)$ curves embracing the critical stress with clearly unsatisfactory results.

Fig. 4 shows the resulting scaling plot of $\sigma(S, T)/\sigma_c(T)$ vs. $|S - S_c|/S_c T^\nu$. The data are seen to collapse on a single branch each for the metallic and insulating side, respectively. The best scaling, as shown, is achieved for $y = 1/\nu z = 0.34$. Together with $\mu = 1.0$ as obtained from Fig. 1 and assuming Wegner scaling $\nu = \mu$ for $d = 3$, we find $z = 2.94$, which is indeed consistent with $\sigma_c \sim T^{1/2} \sim T^{1/3}$ for $T \rightarrow 0$ (see Fig. 2a). Alternatively, we may use Eq. (1) plotting $\sigma(S, T)/|S - S_c|^{\mu}$ vs. $T/|S - S_c|^{\nu}$ (not shown) with the three parameters $S_c, \mu = \nu$ and $z$. The best data collapse is found for $\mu = 1.0 \pm 0.1$ and $z = 2.94 \pm 0.3$, in very good agreement with the values obtained from Fig. 4. Additionally, we note the broad consistency with the earlier concentration tuning data where $\mu = 1.3$ and $z = 2.4$ was inferred [3].

We estimate the error of our combined analysis of the present stress-tuned data to 10% for $\mu$ and $z$. The critical stress is determined with a relative accuracy to better than 0.1 kbar. It is important to note that either $\sigma(0)$ scaling (Fig. 2b) or dynamic scaling (Fig. 4) when taken by itself, may lead to a rather large error in $\mu$ and/or $z$, just because of the ambiguity of determining the critical region. However, the consistent determination of exponents from the combined scaling lends confidence to the values reported here.

The above procedure to determine the conductivity at the critical stress is necessary because $\sigma_c$ does not obey a simple power-law $T$ dependence over the whole $T$ range. Above 100 mK the correction term $dT^w$ (with $d < 0$) comes into play. This is at variance with Si:B where $\sigma_c \sim T^{1/2}$ was observed in the whole range from 60 to 800 mK [15]. On the other hand, a $T^{1/3}$ dependence of $\sigma$ in the vicinity of the MIT has been reported for transmutation-doped Ge:Ga over a large $T$ range [3].

Certainly, the finite-$T$ behavior near the quantum critical point needs closer theoretical scrutiny, in particular since the dynamic scaling is observed up to 800 mK when the correction term to $\sigma_c(T)$ is included. We remark that a simple algebraic $T$ dependence $\sigma_c = a T^2$ yields good dynamic scaling for Si:B [3], clearly leading to less satisfactory scaling in Si:P for any choice of $x$.

In conclusion, we have demonstrated dynamic scaling of stress-tuned Si:P at the metal-insulator transition. The conductivity exponent $\mu \approx 1$ is close to the exponents derived earlier from concentration tuning. However, upon application of stress, the critical range is narrowed to conductivities below $12 \Omega^{-1}\text{cm}^{-1}$. Therefore, it is the absence of appreciable rounding effects in our samples close to the MIT that allows us to determine $\mu \approx 1$ reliably, thus resolving the conductivity exponent puzzle. The temperature dependence of the conductivity starting from the same $\sigma(0)$ value for $T = 0$ is distinctly different for samples under zero stress and under stress. It is predicted that in the region between 15 and 40 $\Omega^{-1}\text{cm}^{-1}$ initially insulating stress-tuned samples will
exhibit a negative slope of $\sigma(T)$, while samples under zero stress in this range are known to have a positive $\sigma(T)$. In view of these differences away from the quantum critical point, the similarity of asymptotic dynamic scaling behavior is particularly noteworthy. A more detailed theoretical treatment which may eventually also account for the effective exponent $\mu \approx 0.5$ for samples above the crossover conductivity $\sigma_{cr}$ is highly desirable.

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