The Observation of Percolation-Induced 2D Metal-Insulator Transition in a Si MOSFET

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By analyzing the temperature (T) and density (n) dependence of the measured conductivity (σ) of 2D electrons in the low density (~ 10¹¹ cm⁻²) and temperature (0.02 - 10 K) regime of high-mobility (1.0 and 1.5 x 10⁵ cm²/Vs) Si MOSFETs, we establish that the putative 2D metal-insulator transition is a density-inhomogeneity driven percolation transition where the density-dependent conductivity vanishes as σ(n) ∝ (n - n_c)ᵖ, with the exponent p ~ 1.2 being consistent with a percolation transition. The ‘metallic’ behavior of σ(T) for n > n_c is shown to be well-described by a semi-classical Boltzmann theory, and we observe the standard weak localization-induced negative magnetoresistance behavior, as expected in a normal Fermi liquid, in the metallic phase.

The so-called two-dimensional (2D) metal-insulator transition (MIT) has been a subject of intense activity and considerable controversy ever since the pioneering experimental discovery of the 2D MIT phenomenon in Si MOSFETs by Kravchenko and Pudalov some fifteen years ago. The apparent MIT has now been observed in almost all existing 2D semiconductor structures, including Si MOSFETs, electrons and holes in GaAs/AlGaAs, and electrons in Si/SiGe heterostructures systems. The basic phenomenon refers to the observation of a carrier density-induced qualitative change in the temperature dependence of the resistivity ρ(n, T), where n_c is a critical density separating an effective ‘metallic’ phase (n > n_c) from an ‘insulating’ phase (n < n_c), exhibiting dρ/dT > 0 (0) behavior typical of a metal (insulator).

The high-density metallic behavior (n > n_c) often manifests in a large (by 25%) decrease in resistivity with increasing temperature in the low temperature (0.05 - 5 K) regime where phonons should not play much of a role in resistivity scattering. The insulating regime, at least for very low (n ≪ n_c) densities and temperatures, seems to be the conventional activated transport regime of a strongly localized system. The 2D MIT phenomenon occurs in relatively high-mobility systems although the mobility values range from 10⁵ cm²/Vs (Si MOSFET) to 10⁷ cm²/Vs (GaAs/AlGaAs) depending on the 2D system under consideration. The 2D MIT phenomenon is also considered to be a low-density phenomenon although, depending on the 2D system under consideration, the critical density n_c differs by two orders of magnitude (n_c ~ 10¹¹ cm⁻² in 2D Si and ~ 10⁹ cm⁻² in the high-mobility GaAs/AlGaAs heterostructures. The universal features of the 2D MIT phenomenon are: (1) the existence of a critical density n_c distinguishing an effective high-density metallic (dρ/dT > 0 for n > n_c) phase from an effective low-density insulating (dρ/dT < 0 for n < n_c) phase; and (2) while the insulating phase for n < n_c seems mostly to manifest the conventional activated transport behavior, the metallic temperature dependence at low (n ≳ n_c) densities is universal in the sense that it manifests a very strong temperature dependence, not seen in standard 3D metals where ρ(T) is temperature independent in the T < 10 K Bloch-Grüneisen transport regime.

The excitement and controversy in the subject arise from the deep conceptual questions associated with the nature of the MIT and the metallic phase. In particular, it is theoretically well-established¹ that a non-interacting (or weakly interacting) disordered 2D electron system is an insulator at T = 0, and therefore it follows that if the 2D MIT is a true T = 0 quantum phase transition (QPT), then the 2D metallic phase, if it survives all the way to T = 0, must necessarily be a novel and exotic non-Fermi liquid phase since it cannot be connected adiabatically to the non-interacting 2D electron system, which is always localized in the presence of any disorder. The alternative possibility is that the metallic phase is allowed only at finite temperatures, and the 2D MIT is not a QPT, but a density-induced crossover from a weakly localized ‘effective’ metallic phase to a strongly localized insulator. These two qualitatively distinct viewpoints have both received support in the literature, and experimental results have been presented claiming support for the QPT and the finite-temperature crossover viewpoints, respectively. Whether the observed 2D MIT is a novel (T = 0) QPT leading to an exotic 2D non-Fermi liquid metallic phase established by interaction effects or is a finite-temperature crossover between an effective metallic phase and the insulating phase is obviously a question of great fundamental importance.

Previous measurements of 2D MIT phenomena in Si MOSFETs have been discussed in terms of quantum critical phenomena. However, for 2D electrons and holes in high mobility GaAs/AlGaAs heterostructures, it has been shown that the 2D MIT can be described as a percolation transition. Thus, a natural question to ask is whether the 2D MIT in Si MOSFETs is really different...
than for GaAs systems, or whether both Si and GaAs 2D systems undergo the same universal percolation-driven transition. The Si MOSFET is different than GaAs systems in that it has much lower mobility and the disorder in Si MOSFETS is thought to be dominated by ‘short-range’ scattering, which is potentially different than for other 2D systems, such as in GaAs where ‘long-range’ scattering may play a larger role. This point has been recently emphasized in the literature and it has been proposed that the physics behind the 2D MIT for Si MOSFETs versus GaAs systems may differ due to differences in mobility and range of the disorder potential (short vs. long-range scattering).

In this article, we provide the first experimental evidence that the MIT for Si MOSFETs is a finite-temperature, density inhomogeneity driven semi-classical percolation transition, and is therefore not a QPT. Our work shows that the 2D MIT is a universal percolation transition for both GaAs and Si, in contrast to claims of a QPT in Si. As mentioned earlier, the 2D MIT in high-mobility GaAs electron and hole systems has already been experimentally demonstrated to be a percolation transition, but our work provides the first compelling evidence supporting the percolation scenario in Si MOSFETs. We also establish that the metallic phase is a conventional Fermi liquid by showing that (1) the measured transport properties in the effective metallic phase qualitatively agree very well with the conclusions of a semi-classical Boltzmann transport theory, taking into account the detailed density and temperature dependence of carrier screening properties, and (2) the expected negative magnetoresistance signature of the conventional weak localization behavior is clearly manifested in the effective metallic phase of our samples.

The two samples used in this study are Si MOSFET structures with a peak mobility of ~ 1.5 × 10^4 cm^2/Vs (sample A) and ~ 1 × 10^4 cm^2/Vs (sample B). For both samples, the 2D electron gas (2DEG) resides at the Si-SiO₂ gate oxide interface, where the SiO₂ thickness is nominally 35 nm for sample A and 10 nm for sample B. The gate oxide is thermally grown in dry O₂ at 900°C on FZ (100)-oriented high-resistivity (> 5 kΩ-cm for sample A and > 100 Ω-cm for sample B, at room temperature) p-type Si wafers. Ohmic contacts to the 2DEG consist of n⁺ Si regions formed by implantation of As; these contacts are not self-aligned, but are instead patterned and implanted before the gate oxide growth. An n⁺ polySi gate, patterned to form a 15 μm × 100 μm Hall bar, is used to induce carriers. The 2DEG resistivity is experimentally determined via standard four-terminal lock-in measurements and the density is calibrated via measurements of the Hall resistivity.

In Fig. 1 we show the density-dependent mobility of samples A and B along with the theoretically calculated mobility curves. Our theoretical calculations include the temperature-dependent finite wavevector screening of the charged impurity Coulomb scattering and the short-range surface roughness scattering at the Si-SiO₂ interface. It is well-known that the long-range charged impurity scattering and the short-range surface roughness scattering dominate respectively the low and the high carrier density regimes of transport in Si MOSFETs. We show Fig. 1a and b together to allow the reader to judge the level of agreement between experiment and theory, which depends on several scattering parameters (e.g. the density and spatial distribution of charged impurity centers in the sample and the height and lateral correlation functions of the interface roughness function). The mobility (µ) first rises steeply with density (n) reaching a maximum at a characteristic density n_m, beyond which µ falls off slowly with increasing n, due to short-range surface roughness scattering at the Si-SiO₂ interface. At low carrier densities (n < 10^12 cm⁻²) however, long-range Coulomb scattering by unintentional random charged impurities invariably present on the insulating oxide side of the Si-SiO₂ interface dominates the 2D mobility, and, as has been emphasized in the literature, all Si 2D MIT behavior manifests itself at low carrier densities (n ~ 10^11 cm⁻²) where the charged impurity scattering dominates transport and the long-range interface roughness scattering is negligible. We emphasize the fact that the 2D MIT phenomenon (i.e. n_c and the density range for the ‘anomalous’ metallic phase with a strongly temperature dependent 2D resistivity) occurs in the density regime n ~ 10^11 cm⁻² which, being substantially below n_m, is completely dominated by the long-range screened Coulomb scattering. This dominance of Coulomb scattering in the 2D MIT physics is crucial for the percolation physics which arises from the nonlinear failure of screening of the long-range Coulombic charged impurity potential, to be discussed below. The short-range surface-roughness scattering, which dominates MOSFET transport for n > 10^12 cm⁻², plays no role in the 2D MIT phenomena since both the
critical density for the transition and the density regime where the strong metallic behavior (i.e. the strong temperature dependence of the 2D conductivity) is observed are well below the operational regime of the short-range surface roughness scattering.

In Fig. 2 we show our measured (Fig. 2(a) - (b)) and calculated (Fig. 2(c) - (d)) temperature and density dependent resistivity ($\rho(T,n)$) for sample A with the maximum mobility of $1.5 \times 10^4$ cm$^2$/Vs (see Fig. 1(a)). The results for sample B are similar, but with a larger value of the critical density, $n_c \sim 2.5 \times 10^{11}$ cm$^{-2}$ (and somewhat weaker temperature dependence), consistent with its lower (and consequently, higher disorder) peak mobility $\sim 1 \times 10^4$ cm$^2$/Vs. The classic 2D MIT behavior is apparent in Fig. 2(a) where $\rho(T)$ for various densities manifests the clear distinction between metallic ($d\rho/dT > 0$) and insulating ($d\rho/dT < 0$) behavior separated (visually) by a critical density $n_c \sim 1.4 \times 10^{11}$ cm$^{-2}$. We note that the temperatures quoted in Fig. 2a and b are those of the cryostat cold finger: although the resistivity continues to evolve below $T \sim 100$ mK (albeit slowly), we cannot claim in this regime ($T < 100$ mK) that the 2D electrons and the cold finger are in thermal equilibrium down to the base temperature of our cryostat (20 mK). The inset in Fig. 2(b) shows in detail the metallic behavior for $n > n_c$, which manifests more than a factor of 2 increase in $\rho(T)$ for $T \sim 0.1 - 7$ K before decreasing slightly at higher temperatures. The strong initial increase in $\rho(T)$ with $T$ arises from the temperature-induced weakening of screening at these low densities as $T/T_F$ increases from 0.01 at low temperatures essentially to 1 at $T \sim 8$ K since $T_F \approx 7.3$ K for $n = 10^{11}$ cm$^{-2}$, (Phonon scattering is unimportant in Si MOSFET for $T < 10$ K.)

Finally, in Fig. 2(c) we show our theoretically calculated $\rho(T,n)$ where the Boltzmann transport is calculated using the screened charged impurity scattering as the only resistive scattering mechanism. Although the ratio of the Coulomb to Fermi energy, $r_c$, can be as large as $\sim 15$ near the MIT for this sample, suggesting that Coulomb interactions could play an important role, we note that the basic features of the experimental metallic phase are well-captured by the screening theory with $\rho(T)$ rising approximately by a factor of 2 initially and then decreasing slightly at higher (lower) temperatures.

Having established the phenomenology of the 2D MIT behavior in Fig. 2, we now come to the nature of the density driven transition itself. We plot in Fig. 3 our measured conductivity $\sigma(n)$ as a function of $n$ to see if a percolation behavior, $\sigma(n) \sim (n-n_p)^\alpha$, where $n_p$, $\alpha$ the percolation transition density and exponent respectively, is manifested. Our fit yields $\alpha \approx 1.20$, $n_p \approx 1.2 \times 10^{11}$ cm$^{-2}$ for sample A and $\alpha \approx 1.24$, $n_p \approx 2.0 \times 10^{11}$ cm$^{-2}$ for sample B. The fits describe $\sigma(n)$ well over nearly two orders of magnitude change in conductivity. The devia
tions of the fit from the data seen at the lowest densities \((n < n_c)\) are expected since our percolation analysis applies only in the metallic regime. At high densities the fit is also expected to deviate since the percolation fit is a critical scaling behavior which is expected to be best for densities close to \(n_p\), and also the role of surface roughness scattering becomes increasingly important at high densities. The fact that our best fit values of \(n_p\) and \(p\) for sample A are almost independent of temperature at low temperatures is a good indicator for the percolation transition being the correct description for the 2D MIT phenomenon shown in Fig. 2. Our numerically extracted best-fit exponent \(p \approx 1.2\) is sufficiently close to the percolation conductivity exponent of 1.31 for us to feel confident that the observed 2D MIT in Si MOSFETs is a density inhomogeneity-driven percolation transition.

In Fig. 4, we show an alternate (and perhaps more appropriate, if the transition is indeed a percolation transition) method of extracting the critical density from a percolation fit, where we hold both the exponent \(p\) and the prefactor \(A\) fixed, and allow only \(n_p\) to vary. We use \(p = 1.31\), the value expected for percolation in 2D, and determine \(A\) from the percolation fit to the \(T = 0.4\) K data, as shown in the inset to Fig. 4, also holding \(p = 1.31\) fixed. If the 2D MIT is indeed a percolation transition, then this method of obtaining \(n_p\) is more appropriate than allowing \(p\) to vary since the exponent is universal and the critical density is not. As seen in the inset to Fig. 4, the fit to our \(\sigma\) vs. \(n\) data with \(p = 1.31\) fixed is very good. As can be seen from the main figure, the extracted \(n_p\) obtained via this method decreases with decreasing temperature, eventually saturating at the lowest temperatures. A fit of the form \(n_p = n_0 + A e^{-b/T}\) is shown as the solid line in the main plot of Fig. 4. The fit yields \(n_p = 1.04 + 1.62 e^{-4.20/T}\). The parameter \(b = 4.2\) K is an effective “energy gap” that can be calculated if the impurity distribution is known. We note that this implies a \(T = 0\) MIT transition density of \(1.04 \times 10^{11}\) cm\(^{-2}\), which is considerably less than the nominal critical density of \(1.4 \times 10^{11}\) cm\(^{-2}\) one would have inferred from the temperature-dependent resistivity behavior in Fig. 2(a). The fact that the temperature-dependent resistivity by itself gives a strong over-estimate of the 2D MIT critical density is already known in the literature.

In Fig. 5 we show our observed weak localization behavior by plotting the expected negative magnetoresistance in the metallic phase as a function of an applied weak magnetic field. The weak localization data in Fig. 5 is fitted to the standard di-gamma function behavior expected of a disordered 2D system:

\[
\Delta \sigma = -\alpha \frac{e^2}{h} g_c \frac{v}{\pi} \left[ \Psi \left( \frac{1}{2} + \frac{\tau_B}{\tau} \right) - \Psi \left( \frac{1}{2} + \frac{\tau_B}{\tau_\phi} \right) \right],
\]

where \(\tau_B \equiv \hbar / 4 e B \sqrt{D}\) and \(D\) is the diffusion coefficient. The behavior is quite normal, explicitly demonstrating that our observed metallic phase \((n > n_c, n_p)\) is indeed the usual weakly localized Fermi liquid metallic phase, and not some exotic non-Fermi liquid \(T = 0\) metal. The observation of the expected weak localization behavior in the 2D metallic phase along with the percolative nature of the transition is strong evidence that the experimental 2D MIT is not a QPT, but a crossover.
Before concluding, we briefly discuss the physics underlying the percolation transition. As emphasized above, the 2D MIT phenomenon occurs in the transport regime dominated by long-range Coulombic charged impurity scattering. It was pointed out some years ago that such a transport regime is susceptible at low carrier densities to a semiclassical percolation MIT since large scale density inhomogeneities (i.e. puddles) could appear in the system due to the nonlinear failure of screening of charged impurities at low carrier densities. One can estimate the density of fixed charge near the Si-SiO$_2$ interface to be about 5 nm inside Si at $n \sim 10^{11} \text{ cm}^{-2}$.

The 2D conductivity percolation exponent is numerically known to be around 1.31, which is close to the exponent value (1.20 for sample A, 1.24 for sample B) we get in our analysis. Finally, we note that the puddles produced by the nonlinear failure of screening of charged impurities in low-density 2D systems have been directly observed in 2D GaAs$_2$ systems.

In conclusion, we have experimentally established that the 2D MIT in Si MOSFETs is a percolation-induced transition driven by the dominance of the long-range charged impurity disorder. At low carrier densities, the failure of linear screening leads to the formation of inhomogeneous puddles in the 2D density landscape, which then produces a semi-classical percolation transition. The nature of the percolation transition and the effective metallic phase is the same in Si MOSFETs and 2D GaAs electron and hole systems. The metallic temperature dependence arises from the strong temperature dependence of screening and the percolation transition arises from the low-density failure of screening. The 2D MIT is therefore a quantum crossover phenomenon, not a QPT, from an effective (weakly localized) metallic phase to a strongly localized insulating phase. The agreement between the percolative conductivity and our experimental work as well as our finding of the usual weak localization effect in our data conclusively rules out quantum criticality in the 2D MIT phenomena. Our work establishes that the 2D MIT is a universal percolation-driven transition, caused by the inhomogeneous density landscape induced by charged impurities at low carrier densities, in both GaAs-based systems and Si MOSFETs (our work). Screening of the charged impurity scattering produces the strong temperature dependence of the apparent metallic phase since low carrier densities automatically imply large values of $T/T_F$, and the eventual failure of screening at still lower densities, where there are just too few carriers to effectively screen the impurity charges, leads to the percolation MIT since the 2D system becomes inhomogeneous due to the formation of puddles.

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