Letter

Anderson localization crossover in two-dimensional Si systems: The past and the present

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Using the Ioffe-Regel-Mott criterion for strong localization crossover in disordered doped two-dimensional (2D) electron systems, we theoretically study the relationships between the three key experimentally determined localization quantities: critical density n_c, critical resistance ρ_c, and sample quality defined by the effective impurity density (as experimentally diagnosed by the sample mobility μ_m at densities much higher than critical densities). Our results unify experimental results for 2D metal-insulator transitions (MITs) in Si systems over a 50-year period (1970–2020), showing that n_c (ρ_c) decreases (increases) with increasing sample quality, explaining why the early experiments in the 1970s, using low-quality samples [$\mu_m \sim 10^3$ cm^2/(V s)], reported strong localization crossover at $n_c \sim 10^{12}$ cm^{-2} with $\rho_c \sim 10^3$ Ω whereas recent experiments (after 1995), using high-quality samples [$\mu_m > 10^4$ cm^2/(V s)], report $n_c \sim 10^{11}$ cm^{-2} with $\rho_c > 10^4$ Ω. Our theory establishes the 2D MIT to be primarily a screened Coulomb disorder-driven strong localization crossover phenomenon, which happens at different sample-dependent critical density and critical resistance values, thus unifying Si 2D MIT phenomena over a 50-year period.

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Introduction. Anderson established in 1958 that a strongly disordered system may localize electrons due to the destructive interference of the electron waves scattering from random disorder [1]. This is one of the cornerstones of modern condensed matter physics as the localization transition is universal in itinerant electron (or bosonic) systems with increasing disorder (or deceasing carrier density) with the system undergoing a metal-insulator transition (MIT) from a metal to an insulator driven by disorder-induced quantum interference leading to electron localization. It was later realized in Refs. [2–4] that in two-dimensional (2D) systems, the localization transition is actually a crossover from an essentially unobservable (except perhaps at extremely low temperatures) logarithmically weakly localized effective metal (i.e., a very weak logarithmically increasing resistivity with decreasing temperature even deep in the metallic phase for any finite system) to an exponentially localized Anderson insulator at some critical density, but this crossover can be very sharp, making the 2D localization crossover appear operationally almost identical to the corresponding Anderson localization in 3D disordered systems where the localization transition is a thermodynamic quantum phase transition. This is known as "weak localization" or "scaling localization" following Ref. [1], stipulating that strictly speaking there is no 2D metal, with the system crossing over from a weakly localized insulator at low disorder to a strongly exponentially localized insulator at large disorder with no phase transition. We ignore the subtle and very small weak localization corrections in this Research Letter and focus on the experimentally reported density-tuned crossover from the higher-density effective metallic phase to a lower-density effective strongly localized phase [5–15]. This crossover is known as the 2D MIT.

This Research Letter explores the theory of 2D localization crossover in 2D Si systems, which has been extensively studied experimentally since the early 1970s [16]. The great advantage of 2D Si systems [e.g., Si metal-oxide-semiconductor field-effect transistors (MOSFETs)] is that the carrier density can be easily tuned in a single sample over a large range just by changing a gate voltage, thus exploring the whole conductor-to-insulator regime from deep in the metallic phase with high conductivity at high density to the strongly localized insulator at low densities where the resistivity basically diverges exponentially at low temperatures. Since metallic conductors and localized insulators are operationally distinguished by the temperature dependence of their low-temperature resistivity, with the metallic (insulating) resistivity increasing as a power law or remaining approximately constant (decreasing exponentially) with increasing temperature, it is easy to experimentally determine the critical crossover density n_c (and the associated critical resistance ρ_c) by identifying the density at which the temperature dependence first manifests an exponentially increasing behavior as temperature is lowered. The ability to tune the carrier density in a single sample (i.e., with a fixed quenched disorder) to obtain n_c and ρ_c has made 2D Si MOSFETs the ideal system to study Anderson localization for almost 50 years, ever since experimental techniques were developed to do transport measurements of Si MOSFETs at cryogenic temperatures. It is therefore no surprise that the very first (circa 1975) disorder-driven and density-tuned Anderson localization from a conducting metallic phase to an activated transport exponentially localized insulating phase with decreasing carrier density was first reported in 2D MOSFETs [17–23]. These early experiments of the 1970s used relatively dirty samples

with $\mu_m \sim 10^3$ cm^2/(V s) deep in the metallic phase, which led to $n_c \sim 10^{12}$ cm^{-2} and $\rho_c \sim 10^3$ Ω [16,24,25]. With improvement in the sample quality and substantial suppression of disorder, however, more recent (circa 2000) localization experiments in Si MOSFETs focused on much higher quality [$\mu_m \sim 10^4$ cm^2/(V s)] samples, typically finding $n_c \sim 10^{11}$ cm^{-2} and $\rho_c \sim 10^4$ Ω [26–31]. The question therefore arises whether the past and the present Si-MOSFET localization experiments observe the same 2D MIT phenomenon or not.

We provide in this Research Letter a unified theory explaining both the past MOSFET experiments of the 1970s in dirty samples and the more recent MOSFET experiments in clean samples within a single theoretical framework, using a physical model of the Anderson localization crossover induced 2D MIT as arising from screened Coulomb disorder [32,33] with decreasing density leading to the strong enhancement of the effective screened disorder which causes the Anderson localization. The large quantitative differences in the values of n_c and ρ_c between the past and the present arise in our theory from the difference in the amount of random disorder (i.e., unintentional background charged impurity density in the system) in the old and the current samples, as reflected by the (at least) one order of magnitude difference in their optimal mobility.

Theory. We use the well-known and extensively used Ioffe-Regel-Mott (IRM) criterion [34] for defining the Anderson localization crossover point:

$$k_F l = 1, \tag{1}$$

where $k_F = (2\pi n/g_v)^{1/2}$ is the 2D Fermi wave vector (where g_v is the possible valley degeneracy and a spin degeneracy of 2 is included) and l is the scattering mean free path given by $l = v_F\tau$, where $v_F = \hbar k_F/m$ is the Fermi velocity and τ is the scattering time. Using the Fermi energy $E_F = (\hbar^2 k_F^2/2m)^{1/2}$, we can rewrite the IRM criterion as

$$E_F\tau = \hbar. \tag{2}$$

The significance of the IRM criterion is that itinerant metallic electrons need to be coherent on the length scale of its wave-packet size, i.e., $1/k_F$, so the minimal condition for metallic transport is the mean free path being larger than the wave-packet size defining the electron: $l > 1/k_F$, which leads to $k_F l = 1$ defining the localization crossover point as a function of disorder (constraining the mean free path) and/or carrier density (constraining the Fermi momentum). The Drude formula defines the resistivity ρ as

$$\rho = \frac{m}{ne^2\tau}. \tag{3}$$

In 2D systems, ρ has the dimensions of resistance and is nothing other than the resistance per square measured in ohms. Expressing the formula above for k_F and E_F in terms of 2D density n, we get from Eq. (3)

$$\rho = \frac{h}{e^2}\frac{k_F l}{g_v}. \tag{4}$$

Thus the 2D resistivity is expressed in units of the resistance quantum, $h/e^2 = 25\,812.8$ Ω, and the nominal IRM criterion, defined by Eq. (1), then gives (assuming $g_v = 1$ or 2) for the critical resistivity ρ_c defining the 2D MIT crossover

$$\rho_c = \begin{cases} h/e^2 \sim 26\ \text{k}\Omega & \text{for a single valley, } g_v = 1 \\ h/2e^2 \sim 13\ \text{k}\Omega & \text{for } g_v = 2 \text{ as it is for Si(100) surface MOSFETs.} \end{cases} \tag{5}$$

Equation (5) decisively shows the theoretical conundrum we face: All Si MOSFETs, totally independent of their disorder content, should have exactly the same critical crossover resistivity of h/e^2 independent of the observed critical density n_c, if the nominal valley degeneracy is lifted (which happens sometimes because of sharp Si-SiO_2 semiconductor-oxide interface breaking bulk symmetries), or $h/2e^2$, if the valley degeneracy is 2 (as it is because of the bulk valley degeneracy of 6 for the Si conduction band). Note that changing the IRM criterion by some factor, e.g., changing $\lambda_F = 1/k_F$ to $\lambda_F = 2\pi/k_F$, the electron wavelength, does not help because it just modifies the critical crossover resistivity by a constant factor (e.g., 2π) without imparting any disorder or carrier density dependence to the universal 2D MIT crossover resistance ρ_c. How can this manifest disorder-independent 2D critical resistance be reconciled with the experimentally observed huge (by an order of magnitude) difference between the reported large ρ_c in current low-disorder samples versus the reported small ρ_c reported in the older high-disorder samples?

We resolve the conundrum by asserting that the IRM criterion should incorporate *not* the transport scattering time (or the transport mean free path), as is universally and uncritically assumed, but the single-particle (sometimes also called "quantum") scattering time or mean free path. The two could be different in principle because the transport quantities must include vertex corrections to the two-particle propagators whereas the single-particle quantities are related to the imaginary part of the single-particle self-energy. The single-particle, τ_q, and the transport, τ_t, scattering times, although being formally different, often turn out to be essentially identical because vertex corrections vanish for isotropic short-range disorder potential, which is often the case. In particular, in 3D electronic materials (e.g., metals) the disorder potential is universally short ranged, and $\tau_t = \tau_q$ as an identity. However, in 2D semiconductors, $\tau_t > \tau_q$ in general, and it is even possible that $\tau_t \gg \tau_q$ in modulation doped 2D structures where the dopant impurities are far away from the carriers [35–37]. In 2D semiconductors, such as Si MOSFET, the main disorder source consists of the random charged impurities (mostly in the SiO_2 oxide layer), which produce a strongly momentum-dependent long-ranged potential with generally weak screening (because of relatively low effective carrier

density and effective mass), and in addition, the charged impurities are often spatially separated from the carriers, making the disorder potential highly anisotropic and thus leading to different values of τ_t and τ_q. The correct quantity to define the IRM criterion (when τ_t and τ_q are different) is obviously the single-particle scattering time (or the single-particle mean free path) since the IRM criterion is a condition on the coherence of the carriers themselves. Obviously, coherence in metallic transport is defined by the magnitude of the single-particle scattering rate staying below its energy E_F. So we now rewrite Eq. (2) as the correct IRM criterion for single-particle coherence defining the localization crossover from coherent metallic transport to Anderson localization:

$$E_F\tau_q = \hbar. \tag{6}$$

We note that the localization criterion is defined by Eq. (6) whereas the resistivity is obviously given by Eq. (3) with τ in Eq. (3) being τ_t by definition:

$$\rho = \frac{m}{ne^2\tau_t}. \tag{7}$$

If τ_q and τ_t are different, it is clear that ρ_c would typically be lower if the IRM criterion involves τ_q ($<\tau_t$), as it should for defining coherent metallic conduction. The expressions for τ_t and τ_q are given by

$$\frac{1}{\tau_t(k)} = \frac{2\pi}{\hbar}\int dz N_i(z)\sum_{k'}|u_{k-k'}(z)|^2 \times (1-\cos\theta_{k,k'})\delta(\epsilon_k-\epsilon_{k'}) \tag{8}$$

and

$$\frac{1}{\tau_q(k)} = \frac{2\pi}{\hbar}\int dz N_i(z)\sum_{k'}|u_{k-k'}(z)|^2\delta(\epsilon_k-\epsilon_{k'}), \tag{9}$$

where $\epsilon_k = \hbar^2k^2/2m$ is the usual parabolic energy dispersion with $m = 0.19$ (in units of free electron mass) being the effective mass, θ is the scattering angle between the incoming and outgoing states ($\boldsymbol{k}$ and $\boldsymbol{k}'$), $N_i(z)$ is the 3D distribution of charged impurities, and $u_{k-k'}$ is the screened Coulomb interaction between a charged disorder and an electron written as

$$u_q(z) = \frac{v_q}{\varepsilon(q)}e^{-qz} = \frac{2\pi e^2}{\varepsilon(q)\kappa q}e^{-qz}. \tag{10}$$

The exponential factor e^{-qz} takes into account a spatial separation of z between the charged impurity layer and the 2D electron layer, and $\varepsilon(q) = 1 + v_q\Pi(q)$ is the random phase approximation static dielectric function, where $v_q = 2\pi e^2/\kappa q$ is the Coulomb interaction with κ denoting the background lattice dielectric constant. $\Pi(q)$ is the 2D static polarizability given by [38]

$$\Pi(\boldsymbol{q}) = -\frac{m}{\pi\hbar^2}\left[1-\Theta(q-2k_F)\frac{\sqrt{q^2-4k_F^2}}{q}\right]. \tag{11}$$

Using Eq. (11), we can rewrite Eq. (10) as

$$u_q(z) = \frac{2\pi e^2}{\kappa(q+q_s)}e^{-qz}, \tag{12}$$

where $q_s = q_{TF}[1-\Theta(q-2k_F)\sqrt{1-(2k_F/q)^2}]$ and $q_{TF} = 2me^2g_v/\kappa\hbar^2$ is the Thomas-Fermi wave vector. Since the scattering rate at the Fermi surface is involved in the zero-temperature transport calculation [i.e., $\tau_t(k_F)$ and $\tau_q(k_F)$], it is easy to see that the momentum transfer $q = |\boldsymbol{k}-\boldsymbol{k}'|$ in Eqs. (8) and (9) is restricted to the range $0 < q < 2k_F$ for our calculations, leading to $q_s = q_{TF}$. Thus the screened Coulomb disorder potential [Eq. (10)] can be equivalently expressed as

$$u_q(z) = \frac{2\pi e^2}{\kappa(q+q_{TF})}e^{-qz}. \tag{13}$$

Note that the $(1-\cos\theta)$ factor in Eq. (8), defining τ_t, arises from vertex corrections in the conductivity, which removes all forward scattering (i.e., $\theta \sim 0$) from the transport scattering rate because scattering in the forward direction does not contribute to the resistivity. By contrast, the $(1-\cos\theta)$ factor is absent in the single-particle quantum scattering rate [Eq. (9)] since all scattering (including the forward direction $\theta \sim 0$) contributes to the quantum decoherence of the single-particle momentum eigenstates. When the disorder potential u_q is purely s-wave, i.e., short ranged and thus independent of scattering momentum q, the $(1-\cos\theta)$ factor drops out, leading to $\tau_t = \tau_q$, as happens in 3D metals, but not necessarily in 2D Si MOSFETs.

For simplicity, and mainly because our interest is a general understanding of how past and present 2D MIT experiments in Si MOSFETs can be reconciled within a unified theory even if they have very different values of ρ_c with $\rho_{c,present} \gg \rho_{c,past}$, we use a minimal two-parameter (n_i and d) model for disorder:

$$N_i(z) = n_i\delta(z-d), \tag{14}$$

where n_i is the 2D random quenched charged impurity density producing the scattering, which is placed at a distance d from the 2D carriers in Si. In reality, of course, $N_i(z)$ is an unknown 3D disorder throughout the Si-MOSFET device, but it is known that the most resistive scattering arises mostly from the random charged impurities invariably present near the interface in the SiO_2 layer [16,39,40]. Therefore the two-parameter impurity model is the minimal sample-independent universal model consistent with the materials physics of all MOSFETs, past and present. We keep the distance d fixed ($d = 5.35$ nm) so that the actual fitting is a minimal one-parameter fitting to the 2D impurity density n_i, or equivalently, to a 3D uniform oxide charge density of $N_i \sim n_i/d$ with d as the centroid of the equivalent 3D impurity distribution. We vary n_i (or N_i) to obtain our results from low-mobility (n_i large) old MOSFET samples to high-mobility (n_i small) recent MOSFETs. The relevant impurity density varies between $n_i \sim 10^{10}$ cm^{-2} and $n_i \sim 10^{13}$ cm^{-2} (between $N_i \sim 1.5\times10^{16}$ cm^{-3} and $N_i \sim 1.5\times10^{19}$ cm^{-3}), consistent with the known charged impurity contents of MOSFETs [16,39,40]. We show our calculated results over a much wider range of n_i.

We also assume, without any loss of generality, a strict 2D approximation for the confined carriers with an effective mass m and a background lattice dielectric constant κ appropriate for the Si-SiO_2 system [16]. In the next section, we present our results based on the theory above, showing the calculated

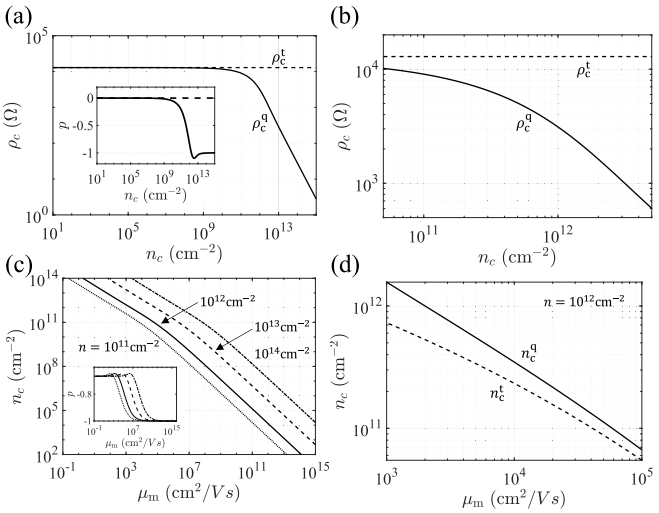

FIG. 1. (a) ρ_c plotted as a function of n_c obtained using the quantum (ρ_c^q, solid line) and transport (ρ_c^t, dashed line) scattering time. The inset in (a) shows the power-law exponent numerically calculated through $p = d \ln \rho_c / d \ln n_c$. (b) Same as (a) but plotted over a typical experimental range of n_c. (c) n_c (obtained using τ_q) plotted as a function of the mobility μ_m deep in the metallic phase (i.e., $n > n_c$) at carrier densities $n = 10^{11}$, 10^{12}, 10^{13}, and 10^{14} cm^{-2}. The inset in (c) shows the corresponding power-law exponent $p = d \ln n_c / d \ln \mu_m$. (d) Plots of n_c obtained using τ_t (dashed line) and τ_q (solid line) at a fixed carrier density $n = 10^{12}$ cm^{-2} over a typical experimental range of μ_m. We use $d = 5.94$ nm throughout with Si(100)-SiO_2 effective band parameters used.

ρ_c, obtained from the modified IRM criterion using τ_q, as a function of the calculated critical density n_c (also obtained from the modified IRM criterion) as well as the calculated n_c as a function of the "maximum" mobility μ_m deep in the metallic phase characterizing the sample quality.

Results. In Figs. 1(a) and 1(b), we show the calculated critical resistivity obtained using τ_t (labeled as ρ_c^t) and τ_q (labeled as ρ_c^q) as a function of n_c. Note that $\rho_c^t \sim 13$ kΩ is given as a constant independent of n_c in agreement with Eq. (5). τ_q exhibits a similar flat behavior at low n_c but starts deviating from τ_t with a strong dependence on n_c at higher $n_c > 10^9$ cm^{-2}, consistent with the experimental findings in Si-MOSFET systems. Figures 1(c) and 1(d) present n_c as a function of the mobility $\mu_m = e\tau_t/m$ with τ_t being calculated at high carrier densities deep in the metallic regime away from the critical density (i.e., $n > n_c$), characterizing the sample quality. In Fig. 1(c), we present several plots of n_c calculated at various carrier densities along with its power-law exponent plotted in the inset. It is worth noting that n_c decreases with increasing μ_m (i.e., increasing sample quality) scaling as $n_c \sim \mu_m^{-p}$ with the calculated exponent, $0.6 < p < 1$, showing a weak density dependence, as observed experimentally. Our theoretical exponent value for p agrees with an empirical finding of p extracted from the recent 2D MIT experimental data [41]. Another experiment already pointed out in 1999 that ρ_c (n_c) increases (decreases) with decreasing sample mobility, in good agreement with our results [42]. Our results clearly show, within one unified theory, that the past and the present 2D MIT experiments in Si MOSFETs manifest identical Anderson localization physics, with the crossover critical density n_c (the crossover critical resistance ρ_c) defining the transition or crossover point increasing (decreasing) with decreasing sample quality (i.e., decreasing μ_m). Thus there is no new physics in the recent 2D MIT experiments for the Anderson localization crossover itself in spite of improvement in the sample mobility over the last 50 years: The transition itself is exactly the same 2D localization crossover approximately defined by the Ioffe-Regel-Mott criterion as was first observed in 1973–1975.

Conclusions. We have shown, using a single unified theory, that 2D MIT crossovers observed in the past and current 2D Si-MOSFET samples essentially arise from the same Anderson localization physics associated with screened Coulomb disorder. We use a realistic model for the Boltzmann transport calculations in 2D Si-MOSFET systems considering screening effects on charged impurities and the separation of the impurity layer away from the 2D electron layer. We find that the IRM criterion incorporating the single-particle scattering time τ_q leads to qualitatively consistent estimates of the critical points (i.e., the critical resistivity ρ_c and density n_c) with the past and current 2D MIT experiments where n_c (ρ_c) decrease (increase) with increasing sample quality, whereas the IRM criterion incorporating the transport-particle scattering τ_t gives sample-quality-independent universal ρ_c, disagreeing with the experimental observations. Our work suggests that the strong localization driven by screened Coulomb disorder is primarily responsible for both past and recent 2D MIT physics in Si systems and there is no new essential physics involved in recent 2D MIT experiments despite the vast sample quality improvement.

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