Exclusion of Quantum Coherence as the Origin of the 2D Metallic State in High-Mobility Silicon Inversion Layers

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The temperature and density dependence of the phase coherence time τ_φ in high-mobility silicon inversion layers was determined from the magnetoresistivity due to weak localization. The upper temperature limit for single-electron quantum interference effects was delineated by comparing τ_φ with the momentum relaxation time τ. A comparison between the density dependence of the borders for quantum interference effects and the strong resistivity drop reveals that these effects are not related to each other. As the strong resistivity drop occurs in the Drude regime, the apparent metallic behavior cannot be caused by quantum coherent effects.

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The apparent "metallic" state in two dimensions (2D) [1] has attracted much attention as it seems to contradict the one parameter scaling theory of Abrahams *et al.* [2]. Following the confirmation of the metallic behavior in several material systems, the question was raised whether the metallic state constitutes a new quantum mechanical ground state, or if the resistivity drop towards lower temperature is based on semiclassical (i.e., noncoherent) effects (see [3], and references therein).

We answer this question for Si-metal oxide semiconductor (MOS) structures, by excluding quantum interference (QI) effects as the origin of the metallic state. This is achieved by determining the phase coherence time τ_φ from the weak localization (WL) behavior and comparing it with the momentum relaxation time τ at different temperatures T and densities n. For $\tau_\varphi > \tau$ (low-T regime), single-electron quantum interference effects occur, whereas for $\tau_\varphi < \tau$ (high-T) they do not, as the coherence time is too short to allow electrons a coherent return to their origin. By comparing the phase coherent regime with the metallic regime, we find that they are not correlated with each other and that metallic behavior exists even without phase coherence. In addition, we determine the temperature where $k_B T = \hbar/\tau$, which marks the threshold for coherent electron-electron (e-e) interaction effects. Again, no correlation with the metallic regime is found.

The T dependence of the phase coherence was already investigated in the early 1980's in Si-MOS structures (see [4,5]). But due to the lack of the metallic state in these low-mobility samples, no appropriate conclusion could be drawn. In recent studies on high-mobility samples with metallic behavior, it was shown that the WL has only small effects on ρ for GaAs/AlGaAs [6] and Si/SiGe [7]. Also for Si-MOS structures in the low ρ (high n) regime, the WL contribution is small and it was shown that spin-orbit coupling is not visible for τ_φ up to 100 ps [8]. But so far, the borders for phase coherence were not determined systematically on a sample with strong metallic behavior in order to decide among the possible underlying mechanisms.

Our investigations were performed on two high-mobility Si-MOS samples Si-15 and Si-43 with peak mobilities of $\mu = 31\,000$ and $20\,000$ cm^2/V s, respectively. Resistivity and Hall measurements were performed with a four terminal ac technique at a frequency of 17.17 Hz.

Figure 1 shows the magnetoresistivity $\rho(B)$ of sample Si-15 for temperatures between 280 mK and 1.59 K at $n = 3.7 \times 10^{11}$ cm^{-2}. The peak in $\rho(B)$ can be fitted by the conductivity corrections arising from single-electron coherent backscattering (weak localization) according to [9]

$$\Delta\sigma_{xx} = -\frac{\alpha g_\nu e^2}{2\pi^2\hbar}\left[\Psi\left(\frac{1}{2}+\frac{a}{\tau}\right)-\Psi\left(\frac{1}{2}+\frac{a}{\tau_\varphi}\right)\right], \tag{1}$$

where Ψ is the Digamma function; $a = \hbar/4eBD$ with B the applied perpendicular magnetic field and D the diffusion coefficient. The values for D and τ were deduced from our Hall and ρ measurements, assuming at first that the linear Drude regime holds (this restriction will be omitted later on). The prefactor $g_\nu = 2$ describes the valley degeneracy for (100) Si-MOS and α depends on the ratio of intravalley to intervalley scattering rates and should lie between 0.5 and 1 [10]. We found values between 0.55 and 0.8, i.e., inside the expected range. The solid lines in Fig. 1 are least square fits of Eq. (1) to the data.

For sample Si-15 the WL peak was followed down to small n of about 1.5×10^{11} cm^{-2}, near the "metal-insulator" transition at $n_c \approx 0.8 \times 10^{11}$ cm^{-2}. At still smaller n, the rising contact resistance decreases the signal-to-noise ratio so that the WL cannot be evaluated any more. Sample Si-43 showed a similar behavior.

The temperature dependence of the phase relaxation time τ_φ and of the momentum relaxation time τ is depicted for sample Si-15 in Fig. 2 for four different n between 1.93×10^{11} and 1.03×10^{12} cm^{-2}. At low

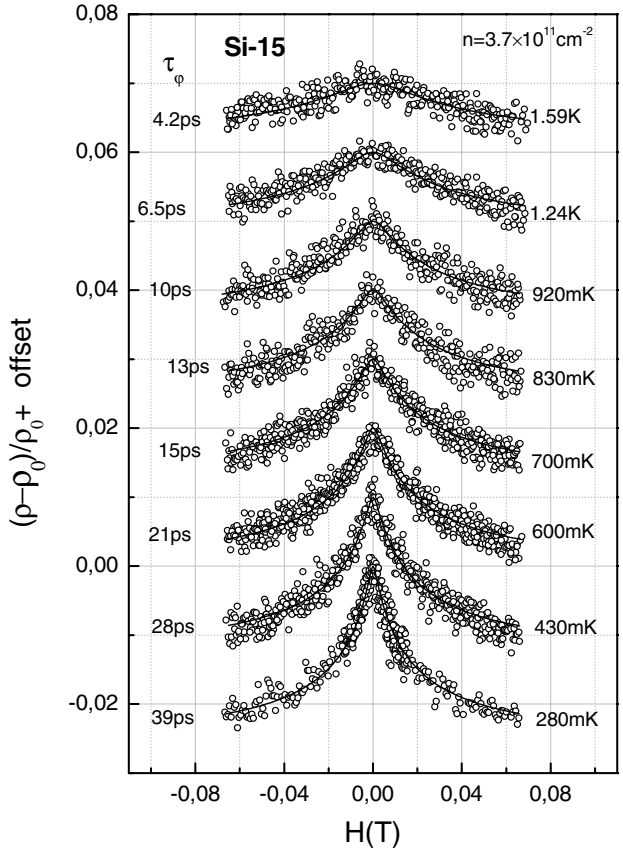

FIG. 1. Change of resistivity versus perpendicular magnetic field for sample Si-15 for eight temperatures at $n = 3.7 \times 10^{11}$ cm^{-2}. The solid lines are fits to weak localization according to Eq. (1).

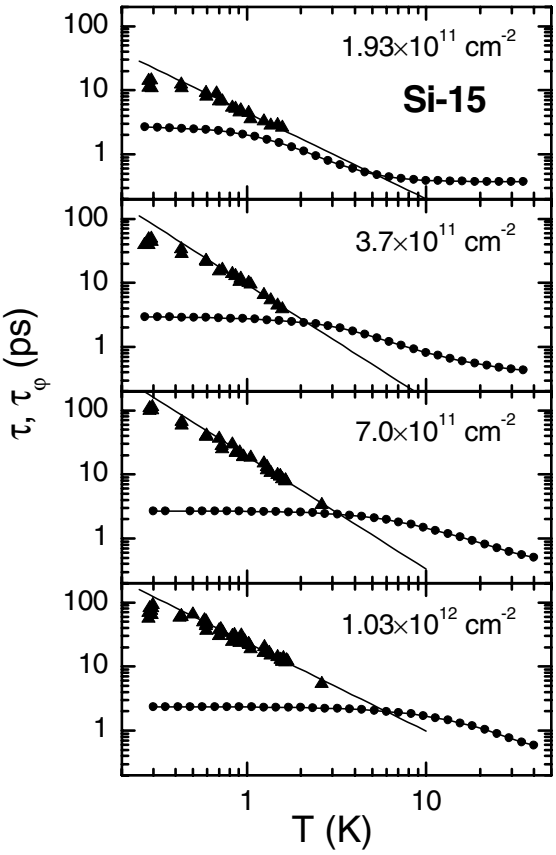

FIG. 2. Experimental temperature dependence of phase coherence time τ_φ (triangles) and momentum relaxation time τ (circles connected by lines) for sample Si-15 at $n = (1.93, 3.7, 7.0, \text{and } 10.3) \times 10^{11}$ cm^{-2}. The thin solid line represents a T^{-p} least mean square fit to the data points.

T, τ_φ exceeds τ by nearly up to 2 orders of magnitude. But since τ_φ strongly decays with temperature, τ_φ and τ cross each other at higher T. When $\tau_\varphi < \tau$ the electrons cannot return to their origin within the phase coherence time and no single-electron QI is possible. Thus the temperature T_q at which $\tau_\varphi = \tau$ defines an upper limit for single-electron quantum interference. This definition is in agreement with our experimental observation that the WL peak vanishes just below T_q. A very similar behavior was found in sample Si-43, where we traced the WL peak for n between 5.4×10^{11} and 3.5×10^{12} cm^{-2} and up to a maximum T of 10.7 K at high n.

For the determination of τ_φ, we used D and τ as calculated from the Hall and ρ measurements, assuming the Drude regime to hold. This is *a priori* not justified, because τ might remain at its "high"-T value and the strong changes in $\rho(T)$ may originate from quantum interference effects. Although we know that weak localization gives only small contributions to $\rho(T)$, there might be additional corrections based on quantum interference. In order to test the above results, we have thus evaluated additionally T_q and τ directly from the WL peak without the use of D, i.e., without assuming the Drude regime to hold. The phase coherence length $\ell_\varphi = \sqrt{D\tau_\varphi}$ follows directly from a fit of the curvature and width of $\rho(B)$ near $B = 0$, independent of D and τ.

The mean free path ℓ is then obtained from the height of the WL peak which is proportional to $\ln(\ell_\varphi/\ell)$. From $\ell_\varphi(T)$ and $\ell(T)$, we find the crossing point T_q at which $\ell_\varphi = \ell$. For $n = 3.7 \times 10^{11}$ cm^{-2} we find, e.g., 2.1 K, which is practically the same as obtained from the crossing of τ_φ and τ, i.e., 2.2 K (see Fig. 2). This shows that the temperature limit T_q does not depend on the assumption that the Drude regime is effective and can be deduced solely from the decrease of the WL peak towards higher T. Knowing ℓ, we can deduce a value for τ from $\tau = \ell/v_F$, with v_F being the Fermi velocity. For example, for $n = 3.7 \times 10^{11}$ cm^{-2}, we obtain a value between 3 and 5 ps at $T = 0.3$ K, depending on the prefactor α. This range for τ is in good agreement with the Drude value of $\tau = 2.85$ ps as deduced from $\rho(T)$ at low T (<2 K) and far away from the high-T value of 0.45 ps (at $T \approx 40$ K in Fig. 2). An estimate of τ exclusively from the weak localization thus leads to the same value as it is obtained assuming the Drude relation $\sigma = ne^2\tau/m^*$. This consistency directly proves that the metallic state indeed obeys Drude behavior.

According to theory, the dependence of τ_φ on conductance and temperature for inelastic e-e scattering in the limit of small momentum transfer (low T) can be described by $\tau_\varphi = \hbar g/k_B T \ln(g/2)$, where g is the dimensionless conductance in units of e^2/h [11]. This relation is strictly valid only for $g \gg 1$. For the case that g becomes of the order of 1, the term $g/\ln(g/2)$ should be substituted by something of the order of unity [12]. By fitting $g/\ln(g/2)$ at $10 \leq g \leq 100$ we obtained the second order polynomial $f(g) = 3.78 + 0.253g - 0.000\,36g^2$ and used this in the above expression.

We find that the calculated $\tau_\varphi(T)$ has a smaller slope than the experimentally determined one. In addition, the calculated values are nearly a factor of 10 larger than the experimentally determined ones, even for $g > 10$. The experimental data can be fitted much better with a T^{-p} law (solid lines in Fig. 2). It seems that the electron system is not in the pure inelastic e-e scattering limit with small momentum transfer. The T^{-p} dependence with $p > 1$ points to a T^{-2} contribution resulting from e-e scattering processes with large momentum transfer (pure metal case) [13]. We find p between 1.1 and 1.7, depending on n, similar to earlier values in Si-MOS (see [4,5] and references therein). For our purpose, it is important that the intersection of the extrapolated T^{-p} dependence with the momentum relaxation time τ gives a well-defined value for the temperature limit T_q for single-electron QI (see Fig. 2).

Figure 3 shows the main feature of the metallic behavior in Si-MOS structures, i.e., the strong drop in $\rho(T)$. The temperature limit T_q for single-electron quantum effects is marked in Fig. 3 by asterisks, connected by a curve to guide the eye. Depending on density, T_q lies between 2 and 10 K. At high density, T_q decreases with decreasing n, but when n drops further T_q returns to higher values. This retrograde behavior is the consequence of the strong decrease of τ in the low n range, which moves the crossing of τ_φ and τ to higher T as can be seen in Fig. 2 for $n = 1.93 \times 10^{11}$ cm^{-2}.

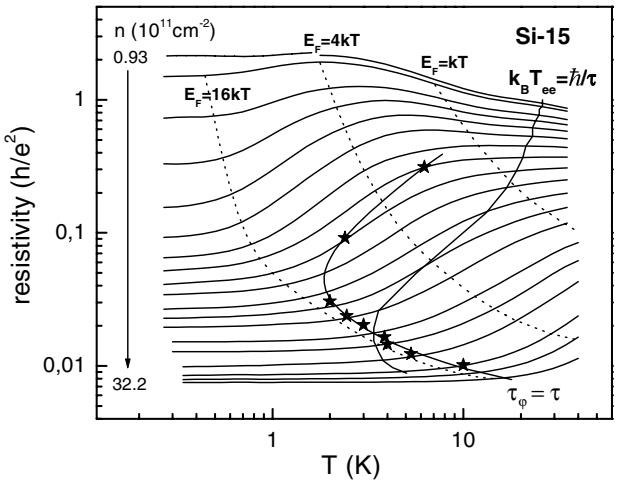

FIG. 3. Temperature thresholds in the ρ vs T plane for Si-15. The asterisks mark the threshold T_q for single-electron quantum interference, and the $k_B T_{ee} = \hbar/\tau$ line indicates the threshold for quantum interference effects due to e-e interaction. Dashed lines mark $E_F/i = k_B T$, with $i = 1, 4$, and 16. Experimental ρ vs T curves are shown for $n =$ (0.928, 0.970, 1.09, 1.18, 1.30, 1.45, 1.64, 1.89, 2.22, 2.64, 3.18, 3.88, 4.79, 6.30, 7.95, 10.2, 15.7, 21.2, and 32.2) $\times 10^{11}$ cm^{-2}.

An important conclusion can be drawn by comparing the overall T dependencies in Fig. 3. The strong drop in $\rho(T)$ occurs for low n between 0.6 and 2 K and shifts with increasing n to much higher T. For the highest n of 3.2×10^{12} cm^{-2} the decrease in ρ lies completely above 10 K. This behavior does not correspond to the observed dependence of the QI threshold T_q which first decreases and then increases with increasing n. For $n > 2.2 \times 10^{11}$ cm^{-2} the strong drop in $\rho(T)$ takes place entirely above the single-electron QI limit T_q and thus must be caused by other effects.

We further indicate the temperature T_{ee} in Fig. 3, which is defined by $\hbar/\tau = k_B T_{ee}$ and gives an upper limit for the occurrence of QI corrections due to the e-e interaction [11]. Again, the run of the temperature limit T_{ee} does not coincide at all with the density and temperature behavior of the strong change in $\rho(T)$. We find again that for large n the strong drop in resistivity is above the quantum correction border T_{ee} and thus the metallic state cannot be caused by e-e induced QI effects either.

As there is no room for QI effects at high densities, the strong $\rho(T)$ drop has to be generated by semiclassical effects. But even at smaller densities, where the resistivity drop is quite similar, it is not expected that its origin is suddenly changing from non-QI to QI. A strong influence of semiclassical effects should extend even to much lower densities.

On the other hand, negative magnetoresistance due to weak localization was found for $T < T_q$ at all densities, demonstrating the existence of small single-electron QI effects at low T. This behavior is in contradiction to the suggested superconductivity of the metallic state [14], where no single-electron QI is expected.

We also indicate the relations $E_F = k_B T$, $E_F = 4k_B T$, and $E_F = 16k_B T$ in Fig. 3, which are related to electron degeneracy. It is worth noting that the bulk of the resistivity changes takes place along the $E_F = 4k_B T$ line for a very large density range which in itself favors a semiclassical explanation for the strong resistivity drop. In addition, we find that the equality $E_F = 16k_B T$ is relatively close to the low-T saturation of $\rho(T)$, although small changes persist to even lower T.

As the strong $\rho(T)$ drop at high densities is caused by semiclassical effects, we discuss several mechanisms. For p-Si/SiGe samples, with small changes of about 10% in $\rho(T)$, it has been shown that the metallic behavior can be explained by temperature dependent screening effects for impurity scattering [15]. But as in the Si-MOS system, the observed changes in $\rho(T)$ amount up to a factor of 10, and the question is how large can the contribution

of screening be. Das Sarma and Hwang have calculated numerically that indeed changes by an order of magnitude may occur in $\rho(T)$ [16]. Very recent calculations of Gold [17] indicate that exchange/correlation and multiple scattering effects dominate the screening behavior for small n and that the large ratio of up to 10 in $\rho(B_c)/\rho(B = 0)$ in parallel magnetic field can also be explained, where B_c is the field for complete spin polarization [18]. In agreement with the expected screening behavior, a linear T dependence in $\rho(T)$ has been observed in high-mobility Si-MOS samples in the intermediate T range at low n [19].

The scattering of electrons at charged hole traps in the oxide layer of Si-MOS is also able to explain a strong T and B dependence of ρ in the frame of semiclassical effects [20]. The filling of hole traps and thus the efficiency of scattering depends strongly on the Fermi energy E_F which depends on n and T. The low-T saturation of ρ in the metallic regime is in this model an interplay between the neutralization of the charged traps (for E_F above trap energy) and the T-independent scattering at low temperatures by surface roughness and residual impurities. In a recent paper, it was shown that the density of defect states on the Si/SiO_2 interface has a large influence on the $\rho(T)$ behavior of the system [21].

As a third mechanism also band splitting may give rise to strong variations in $\rho(T)$. In p-GaAs/AlGaAs, temperature dependent interband scattering [22] and anomalous magneto-oscillations [23] have been observed in the metallic state. These effects are related to the strong spin-orbit interaction together with the inversion asymmetric confinement potential, which induces a splitting of the upper valence band. But spin-orbit interaction is very weak in Si-based structures [24] and does not lead to large changes in $\rho(T)$ in our system. Recently, a small valley splitting at magnetic fields $B \rightarrow 0$ was extracted from precise Shubnikov–de Haas investigations [25]. It was found that the mobilities in the two valleys are very similar and thus cannot cause large changes in $\rho(T)$ either.

For the large range of carrier densities investigated in our Si-MOS structures, we attribute the strong metallic decay of $\rho(T)$ both to carrier screening and impurity scattering effects. The metallic state is observed over nearly 2 orders of magnitude in electron density and thus the relative strength of these different mechanisms will vary. Valley splitting is ruled out as the mechanism causing the large drop in $\rho(T)$.

In conclusion, we have answered the fundamental question about the origin of the metallic state by showing that the strong resistivity drop exists without the presence of quantum effects. The borders for phase coherence were deduced from the temperature dependence of the weak localization at different densities. For densities above 2.2×10^{11} cm^2, the decrease of the resistivity into the metallic regime takes place in the absence of phase coherence. Also disorder induced quantum interference effects due to electron-electron interaction cannot be the origin of the metallic state as the boundary $\hbar/\tau = k_B T_{ee}$ is not related with the resistivity drop either. Thus semiclassical effects are responsible for the low resistivity state over a very large carrier density range in the Si-MOS system, where the temperature dependence of the resistivity is the strongest of all 2D systems.

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