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Binhui Hu, M. M. Yazdanpanah, B. E. Kane, E. H. Hwang, and S. Das Sarma
Phys. Rev. Lett. 115, 036801 — Published 13 July 2015
DOI: 10.1103/PhysRevLett.115.036801
Strongly metallic electron and hole 2D transport in an ambipolar Si-vacuum field effect transistor

Binhui Hu,1,2 M. M. Yazdanpanah,1,2 B. E. Kane,1,2 E. H. Hwang,2,3,4 and S. Das Sarma2,3

1Laboratory for Physical Sciences, University of Maryland at College Park, College Park, MD 20740
2Joint Quantum Institute, University of Maryland, College Park, Maryland 20742, USA
3Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111
4SKKU Advanced Institute of Nanotechnology and Department of Physics, Sungkyunkwan University, Suwon 440-746, Korea

(Dated: May 4, 2015)

We report experiment and theory on an ambipolar gate-controlled Si(111)-vacuum field effect transistor (FET) where we study electron and hole (low-temperature 2D) transport in the same device simply by changing the external gate voltage to tune the system from being a 2D electron system at positive gate voltage to a 2D hole system at negative gate voltage. The electron (hole) conductivity manifests strong (moderate) temperature dependence with the conductivity decreasing by a factor of 8 (2) between 0.3 K and 4.2 K with the peak electron mobility (∼18 m²/Vs) being roughly 20 times larger than the peak hole mobility (in the same sample). Our theory explains the data well using RPA screening of background Coulomb disorder, establishing that the observed metallicity is a direct consequence of the strong temperature dependence of the effective screened disorder.

It is now well-established that, quite generically, “high mobility” and “low-density” semiconductor-based effectively metallic 2D systems can manifest anomalous low temperature “metallic” (i.e., \( d\sigma/dT < 0 \) with \( \sigma \) being the 2D conductivity) transport behavior, where a modest variation in temperature \( T \approx 0.1K - 4K \) could decrease \( \sigma \) by a large amount, with variations in \( \sigma(T) \) by as large as a factor of ∼2 observed in Si MOSFET based 2D electron systems (2DES) [1] and GaAs-based 2D hole systems (2DHS) [2] in a temperature regime \( 0.1K - 4K \) where phonons are inactive due to the Bloch-Grüneisen (BG) suppression of phonon occupancy. This strong metallic temperature dependence (the precise quantitative definition of “high-mobility” and “low-density” is materials dependent and varies from system to system [3]) in 2D semiconductor structures is in sharp contrast with 3D metals where, at low temperatures (\( \lesssim 10K \)), the conductivity typically saturates to a disorder-dependent (and temperature-independent) constant \( \sigma_0 \) as the system enters the BG phonon scattering regime with \( \sigma(T) \approx \sigma_0 - O(T^{4-6}) \). By contrast, the observed anomalous \( \sigma(T) \) in high-mobility and low-density 2D semiconductor systems appears to follow a leading-order linear temperature dependence, with \( \sigma(T) \approx \sigma_0 - O(T) \) over a wide temperature range \( 0.1K - 4K \) although eventually (for \( T < 50 \text{ mK} \) \( \sigma(T) \) saturates (or manifests weak localization behavior[4]), perhaps because of electron heating effects invariably present in semiconductors.

In the current work we report three remarkable new results on the anomalous 2D metallic behavior by combining experiment and theory: (i) we present the first experimental results on the 2D metallic behavior in an ambipolar system where the metallic temperature dependence in the conductivity is separately observed for both 2DES and 2DHS in the same device simply by changing an external gate voltage (we mention that low-mobility ambipolar Si 2D devices have earlier been reported in the literature[5] without any observation of the temperature-dependent metallic transport, which is the focus of our study); (ii) our observed ‘metallicity’ (i.e., the temperature-induced fractional change in the conductivity) is an unprecedented factor of 8 (2) in the 2DES (2DHS) for \( T = 0.3 - 4 \text{ K} \) range and carrier density \( \sim 3 \times 10^{11} \text{ cm}^{-2} \) – this is by far the largest temperature-induced fractional change in the metallic conductivity ever reported in any non-superconducting system in such a small temperature window – for example, earlier-studied 2D Si ‘metallic’ systems in the literature [6] show at most a factor of 3 change in the conductivity in the same temperature window; (iii) we explain our observations qualitatively by calculating the temperature and density dependent RPA-Boltzmann conductivity using a realistic model of screened Coulomb disorder where the main difference between 2DES and 2DHS arises from the effective valley degeneracy being 6 and 1 respectively by virtue of the qualitatively different band structures in the conduction and the valence band of the Si(111) ambipolar FET structure used in our experiment – this leads to the screened effective disorder in the 2DES being much weaker (and much more strongly temperature-dependent) than in the 2DHS, although both see exactly the same bare disorder, explaining the remarkable difference in the mobility and the temperature dependence in the two cases.

The ambipolar FET device (we have actually studied several such devices with similar results) we study is a high-purity and high-mobility hydrogen-terminated atomically flat (and nominally undoped) Si(111) struc-
the usual Si-SiO₂ characterization of such Si-vacuum FETs (in contrast to aging through a vacuum barrier. Details of fabrication and tuning, where the electrons (holes) are induced near the surface) roughness scattering, which dominates 2D carrier transport in standard Si-SiO₂ MOSFETs [16, 17] and in the GaAs-based gated ambipolar devices [12, 13], plays (at best) a minor role in the Si-vacuum 2D structures (similar to the corresponding situation in GaAs-based modulation-doped high-mobility 2D systems [18]) due to the atomically flat nature of our high-quality Si(111) surface; (vi) the main density regime of interest (≥ 1.5 \times 10^{11} cm⁻²) for the study of the 2D effective metallic behavior has \( k_p l > 1 \) (Fig. 2(a)) for both electrons and holes (with \( k_F l \) being Fermi wave vector and mean free path, respectively) implying that a Boltzmann theory based transport theory should work well for both the 2DES and the 2DHS existing in our ambipolar device; (vii) the threshold carrier density (obtained by extrapolating the measured electron or hole Hall density to zero conductivity in Fig. 1(a)–(d)) is almost the same for the 2DES and the 2DHS with the hole system having only a very small amount of (≥ 8 \times 10^9 cm⁻²) higher surface charge states populated by the gate, indicating the very high quality of the sample and that the two systems have almost iden-
leaving a ground state valley degeneracy of \( g_v = 6 \) which lifts four of the valleys higher in energy in the literature [16] where \( g_v = 6 \) likely because of uniaxial interface strain at the Si-SiO\(_2\) most low mobility Si-SiO\(_2\) surface is consistent with earlier experimental re-

In Fig. 2(c) we show our theoretically calculated \( \sigma(n,T) \) for the 2DES to be compared with the corresponding experimental data in Fig. 2(b) whereas Fig. 2(a) shows that for density \( > 10^{11} \text{cm}^{-2} \) the Boltzmann theory should be valid as \( k_{FL} \gg 1 \) applies for the experimental conductivity. The finite temperature 2D Boltzmann theory has already been described by us in details in our earlier work on Si MOSFETs [3, 19], and we only mention that the results shown in Fig. 2(c) use finite-temperature and finite-wave vector RPA screening [20] of the background disorder which is taken to be un-

We note that although theory and experiment agree reasonably well qualitatively using \( g_v = 6 \) (and even quantitatively for density above \( 1.3 \times 10^{11} \text{cm}^{-2} \)) in Fig. 2, we have not attempted any quantitative fitting because the precise disorder parameters are unknown in the experiment. (We mention that using \( g_v = 2 \) in the theory gives results in qualitative and quantitative disagreement with the experimental data for the 2DES.)

In Fig. 3 we show the theoretical results for two temperatures (\( T = 0.3 \text{K} \) and \( 4.2 \text{K} \)) for both 2DES (both \( g_v = 2, 6 \) are shown for the sake of comparison in Fig. 3(a)) and 2DHS (only \( g_v = 1 \) is shown since the Si valence band has no valley degeneracy). The theory reproduces all the key features of the experimental data provided \( g_v = 6 \) (1) is used for the 2DES (2DHS). In particular, there is a very large (\( \sim \) a factor of 20) difference in the 2DES and 2DHS mobilities although both see identical disorder. We have checked explicitly that this mobility difference arises mainly from the different valley degeneracies in the two cases – for example, changing the electron or hole effective mass does not modify the results much whereas changing the valley degeneracy for either electrons or holes has a huge effect. The theory also reproduces the much stronger temperature dependence of the 2DES conductivity compared with the 2DHS case, again arising primarily from the valley degeneracy difference. Finally, we show in Fig. 3(b) the calculated exponent (with \( \sigma \sim n^x \)) for 2DES and 2DHS at \( T = 0.3 \text{K} \) and \( 4.2 \text{K} \), finding for the 2DES (with \( g_v = 6 \)) the exponent \( x = 1.3 \) and \( 2.2 \) for \( T = 0.3 \text{K} \) and \( 4.2 \text{K} \), respectively, and for the 2DHS (with \( g_v = 1 \)) \( x = 1.0 \) and \( 1.1 \) for \( T = 0.3 \text{K} \) and \( 4.2 \text{K} \) respectively. These theo-

FIG. 2. (a) Calculated \( k_{FL} \) using experimental conductivity with different values of \( g_v \). (b) The experimentally measured conductivity as a function of temperature for several electron densities, \( n = 0.85, 0.91, 0.99, 1.15, 1.30, 1.46, 1.61, 1.92, 2.39, 3.17, 3.94, 4.72, 5.49, 6.12 \times 10^{11} \text{cm}^{-2} \) (bottom to top). (c) Calculated conductivity in the presence of ionized channel impurities and surface roughness for electron densities \( n = 1.3, 1.5, 2.0, 3.0, 4.0, 4.5, 5.5, 6.0 \times 10^{11} \text{cm}^{-2} \) (bottom to top). Inset in (c) shows the experiment/theory results together for carrier densities \( n = 1.3, 1.46, 1.61, 1.92, 2.39, 3.17, 3.94, 4.72, 5.49, 6.12 \times 10^{11} \text{cm}^{-2} \) demonstrating reasonable agreement.

We emphasize that all our theoretical results assume the same bare disorder for both 2DES and 2DHS and incorporate all the realistic microscopic details.[16] We note that the
small threshold difference of $8 \times 10^8 \text{ cm}^{-2}$ surface charge density between the 2DES and the 2DHS has no quantitative effect on our theoretical results.

Before concluding, we provide a simple intuitive understanding of the theory which successfully explains the data. At first, the conductivity data appear intriguing because of the huge difference in the quantitative behavior of the conductivity for 2DES and 2DHS in the same sample. Basically, this difference arises from the substantial difference in the effective screened disorder seen by the two kinds of carriers (electrons or holes) in the same ambipolar device because of the large difference in the conduction/valence band structure giving rise to $g_e = 6$ (electrons)/$1$ (holes). The crucial dimensionless quantities [3, 14] determining both the mobility and the temperature dependence of the conductivity are $q_{TF}/k_F$, where $q_{TF}$ and $k_F$ are the 2D Thomas-Fermi and Fermi wave vectors, and $T/T_F$, where $T_F (= E_F/k_B)$ is the Fermi temperature ($E_F$ is the Fermi energy). We emphasize that the dimensionless interaction strength parameter $r_s \propto m/\sqrt{n}$ is in fact larger for the hole system than the electron system, and is not relevant in controlling the temperature dependence with the relevant control parameter being $q_s (= q_{TF}/k_F) \sim g_e^{-1/2} r_s$, which is much larger for the 2DES compared with the 2DHS in our system. We assume that only screened Coulomb disorder (and not phonon scattering) determines the conductivity in the 2D Si system as is expected in the $T = 0.3 - 4.2$ K range.[16] The constraint on $T/T_F$ is simply that it should not be too small in the experimental temperature window for $\sigma(T, n)$ to have strong $T$-dependence. It is easy to see that $T_F^{(h)}/T_F^{(e)} \sim 3$ using $g_e^{(e)} = 6, \ g_e^{(h)} = 1$ and the respective electron/hole effective masses. (The hole effective mass is known to increase from 0.3 to 0.36 in the experimental carrier density range[22], but this does not affect our theory in any quantitative manner.) Thus, the fractional conductivity change, being linear in $T/T_F$ at low temperatures [20], is expected to be much larger for 2DES than for 2DHS in a given temperature range simply by virtue of the electron valley degeneracy being six times larger! But this is only a part of the explanation. The central quantity of key importance in the theory [3, 19, 20] is the dimensionless screening strength $q_s = q_{TF}/k_F$ which determines both the overall magnitude of the mobility as well as the magnitude of the temperature dependence. It is easy to see that $q_s^{(e)}/q_s^{(h)} = (m_e/m_h)(g_e^{(e)}/g_e^{(h)})^{1.5} \sim 8$, which implies that the effective screening is much stronger for the 2DES than for the 2DHS, leading to the conclusion that the mobility ratio for the 2DES compared with 2DHS goes approximately as $(m_e/m_h)(g_e^{(e)}/g_e^{(h)})^2 \sim 35$, whereas the exact numerical calculation gives more a factor of 20 difference since the system is not strictly in the $q_s \gg 1$ and/or $T/T_F \ll 1$ limit that these analytical approximations assume. Similarly, the simplest analytical theory predicts that the temperature-induced fractional conductivity change should go as $(q_s^{(e)}/q_s^{(h)})(T_F^{(h)}/T_F^{(e)}) \sim 20$ assuming that $q_s \gg 1$ and $T/T_F \ll 1$ for both 2DES and 2DHS. Since these strong-screening and low-temperature conditions are not obeyed in the experiment, the realistic difference in the temperature-dependent conductivity, as obtained in our numerical results, is around a factor of 4. For the theoretical details we refer to the existing literature.[3, 19, 20]

In conclusion, we report the first experimental observation of very strong metallic temperature dependence of 2D conductivity in both electrons and holes in an ambipolar Si(111) system, with the electron (hole) conductivity changing by a factor of 8 (2) at a density of $3 \times 10^{11}$ cm$^{-2}$ for a temperature change from 0.3 K to 4.2 K with the electron mobility being 20 times larger than the hole mobility. We provide a theoretical explanation for the data using an RPA-Boltzmann transport theory assuming background screened Coulomb disorder as the primary scattering mechanism. Our work conclusively shows the dominant role of valley degeneracy in determining 2D transport through carrier screening of Coulomb disorder and explains the main difference between the electron and the hole conductivity as arising from the factor of six difference in their valley degeneracy. In particular, we find that the dimensionless parameter $q_{TF}/k_F$ and not the so-called $r_s$-parameter with $r_s \sim m/\sqrt{n}$ controls the strength of metallicity in the anomalous 2D metallic phase of semiconductor systems.

This work is supported by LPS-CMTC. Part of this work was performed at the NIST Center for Nanoscale Science and Technology, and the support of the Maryland NanoCenter through its FabLab is also acknowledged.
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