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# Investigation of Mobility Limiting Mechanisms in Undoped Si/SiGe Heterostructures

X. Mi,<sup>1</sup> T. M. Hazard,<sup>1</sup> C. Payette,<sup>1</sup> K. Wang,<sup>1, \*</sup> D. M. Zajac,<sup>1</sup> J. V. Cady,<sup>1</sup> and J. R. Petta<sup>1, 2</sup>

<sup>1</sup>Department of Physics, Princeton University, Princeton, NJ 08544, USA

<sup>2</sup>Department of Physics, University of California, Santa Barbara, CA 93106, USA

We perform detailed magnetotransport studies on two-dimensional electron gases (2DEGs) formed in undoped Si/SiGe heterostructures in order to identify the electron mobility limiting mechanisms. By analyzing data from 26 different heterostructures we observe a strong correlation between the background oxygen concentration in the Si quantum well and the maximum mobility. The highest quality wafer supports a 2DEG with mobility  $\mu = 160,000 \text{ cm}^2/\text{Vs}$  at a density  $n = 2.17 \times 10^{11}/\text{cm}^2$ and exhibits a metal-to-insulator transition at a critical density  $n_c = 0.46 \times 10^{11}/\text{cm}^2$ . We extract a valley splitting  $\Delta_v \sim 150 \ \mu\text{eV}$  at a magnetic field B = 1.8 T. These results provide evidence that undoped Si/SiGe heterostructures are suitable for the fabrication of few-electron quantum dots.

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# I. INTRODUCTION

The development of silicon quantum devices has gained considerable momentum due to reports of exceptionally long quantum coherence times<sup>1</sup>. Its naturally abundant isotope, <sup>28</sup>Si, carries zero nuclear spin, reducing hyperfine-induced spin dephasing<sup>2-4</sup>. Small spin-orbit coupling is also beneficial for spin qubits<sup>4</sup>. Following work in GaAs quantum dots, early experimental efforts were made towards fabricating Si quantum dots in modulation-doped Si/SiGe heterostructures, where the n-type dopant layer is separated from the Si quantum well (QW) by a setback distance ranging from 5 to 20 nm<sup>5-8</sup>. Doped devices were challenging to operate in the few-electron regime, unstable<sup>8</sup>, and sometimes suffered from gate leakage<sup>5,7</sup>.

It is now widely accepted that the elimination of the n-type dopant layer decreases the Coulomb disorder in the QW, and reduces hysteresis and gate leakage<sup>9,10</sup>. Recent experiments on quantum dots made in undoped Si/SiGe QWs<sup>9–12</sup> have consistently reached the single-electron regime and demonstrated inhomogeneous spin dephasing times  $T_2^* = 360$  ns in naturally abundant Si, a substantial increase compared to GaAs spin qubits<sup>3,12</sup>. Further improvement of the Si/SiGe QW system may be feasible if the remaining mobility limiting mechanisms are identified<sup>13,14</sup>.

The dominant scattering sources can be identified from measurements of the carrier mobility  $\mu$  as a function of 2DEG charge density n, and measurements of the quantum lifetime  $\tau_q^{13,15}$ . For example, scattering from remote impurities<sup>13</sup> is predicted to result in a power-law dependence  $\mu \propto n^{1.5}$ . Such experiments have been extensively performed for GaAs/AlGaAs heterostructures<sup>16–19</sup>, Si MOSFETs<sup>20</sup>, and doped Si/SiGe heterostructures<sup>21–23</sup>. Similar measurements on undoped Si/SiGe heterostructures tures are scarce<sup>23,24</sup>.

To thoroughly investigate the mobility limiting mechanisms in undoped Si/SiGe QWs, we report a series of systematic magnetotransport measurements. By examining 26 different heterostructures, we identify a strong correlation between background oxygen concentration in the QW and maximum mobility. These results indicate that significant enhancements in Si/SiGe mobility might be obtained through more careful control of background contamination during heterostructure growth.

# II. SILICON GERMANIUM HETEROSTRUCTURES

The samples were grown at Lawrence Semiconductor Research Laboratory using chemical vapor deposition [Fig. 1(a)]. Relaxed buffers of  $Si_{1-x}Ge_x$  are first grown on 6 inch diameter Czochralski process Si substrates with 10-20 ohm-cm resistivity, varying x from 0 to 0.3 over a thickness of 3  $\mu$ m. A 1  $\mu$ m thick layer of Si<sub>0.7</sub>Ge<sub>0.3</sub> is grown on the virtual substrate before it is polished. The relaxed buffer substrate has threading dislocation densities on the order of  $10^6/\text{cm}^2$ , as determined by crosssectional transmission electron microscopy. The wafers are completed by growing a 225 nm thick  $Si_{0.7}Ge_{0.3}$  layer, followed by a strained Si QW, a  $Si_{0.7}Ge_{0.3}$  spacer layer and a protective Si cap. All heterostructure layers are grown at a temperature of 650 °C. The  $Si_{1-x}Ge_x$  layers are grown with  $H_2SiCl_2$  and  $GeH_4$  at a rate of 60 - 65nm/min. The Si Cap is grown with H<sub>2</sub>SiCl<sub>2</sub> at a rate of 2 nm/min and the Si QW is grown with  $SiH_4$  at a rate of 9 - 10 nm/min. We investigate heterostructures with Si cap thicknesses of 2 nm and 4 nm,  $Si_{0.7}Ge_{0.3}$  spacer layer thicknesses h = 20 nm, 30 nm, 40 nm and 50 nm, and Si QW thicknesses of 5 nm, 8 nm and 11 nm.

Hall bars are fabricated on each of the 26 wafers, with the geometry shown in Fig. 1(b). We first use atomic layer deposition to grow an Al<sub>2</sub>O<sub>3</sub> gate dielectric on top of the Si cap. We then evaporate Cr/Au on top of the Al<sub>2</sub>O<sub>3</sub> to form a top gate. A positive dc bias is applied to the top gate to accumulate electrons in the QW and a 0.1 mV, 17 Hz ac voltage excitation is applied between the S and D ohmic contacts. The longitudinal voltage,  $V_{\rm xx}$ , Hall voltage,  $V_{\rm xy}$ , and sourcedrain current,  $I_{\rm SD}$ , are simultaneously measured using standard ac lock-in techniques. The 2D longitudinal re-



FIG. 1: (a) Heterostructure growth profile. (b) Top view of the Hall bar device. The gold region marks the area covered by the top gate. The other six square pads are <sup>15</sup>P implanted regions which form Ohmic contacts to the electron gas. The Hall bar dimensions are  $W = 170 \ \mu\text{m}$  and  $L = 375 \ \mu\text{m}$ . (c) A typical "turn-on" curve of the device at T = 0.35 K showing  $I_{\rm SD}$  as a function of  $V_{\rm G}$ . The threshold voltage is  $V_{\rm T} = 0.45$ V. Inset shows n for  $V_{\rm G} > V_{\rm T}$ , before saturation. Dimensions and data shown in (a) and (c) are for Wafer No. 16.

sistivity,  $\rho_{\rm xx} = (V_{\rm xx}/I_{\rm SD})(W/L)$ , and Hall resistivity,  $\rho_{\rm xy} = (V_{\rm xy}/I_{\rm SD})$  are calculated from the measured voltages and currents. Density, n, and mobility,  $\mu$ , of carrier electrons are calculated according to the Hall formulas  $n = B/(e\rho_{\rm xy})$  and  $\mu = (1/B)(\rho_{\rm xy}/\rho_{\rm xx})$ .

Figure 1(c) displays a typical "turn-on" curve of the Hall bar devices. Zero current flow is observed below a threshold top gate voltage  $V_{\rm T} = 0.45$  V. For  $V_{\rm G} > V_{\rm T}$ , current starts to flow and we observe a linear increase in n with a slope of  $dn/dV_{\rm G} = 3.96 \times 10^{11}/{\rm cm^2/V}$ . Using relative permittivities  $\epsilon_r = 9$  for Al<sub>2</sub>O<sub>3</sub> and  $\epsilon_r = 13.1$  for Si<sub>0.7</sub>Ge<sub>0.3</sub>, we calculate  $dn/dV_{\rm G} = 4.00 \times 10^{11}/{\rm cm^2/V}$ , which is within 1 % of the experimental value. At even higher values of  $V_{\rm G}$  (data not shown), electrons start to accumulate at the Al<sub>2</sub>O<sub>3</sub>/Si cap interface, screening the QW from any further increase in  $V_{\rm G}$ . This causes a saturation of the electron density at a constant value of 8.0  $\times 10^{11}/{\rm cm^2}$  for  $V_{\rm G} > 2.5$  V<sup>25</sup>.

#### III. CHARACTERIZATION AT T = 4.2 K

Hall bars are first measured at T = 4.2 K and B = 0.1 T, below the onset of Shubnikov-de Haas (SdH) oscillations. Figure 2(a) shows the spacer layer thickness h for each of the 26 wafers, along with the Si cap thickness and QW width. Recent studies of undoped Si/SiGe structures have shown that remote impurity scattering typically dominates in the low electron density regime, whereas both remote impurities and interface roughness dominate at higher electron densities<sup>23,24</sup>. It is therefore

helpful to examine electron mobilities in both regimes. Electron mobilities are plotted in Fig. 2(b) for  $n_{\rm H} = 7.0 \times 10^{11}/{\rm cm}^2$  and in Fig. 2(c) for  $n_{\rm L} = 2.1 \times 10^{11}/{\rm cm}^2$ . Surprisingly, the mobilities show a nearly monotonic increase with wafer number, despite the large variation in heterostructure parameters throughout this series of wafers. On top of this trend, abrupt dips in the mobility are observed at Wafer No. 20 and 26.

Secondary ion mass spectrometry (SIMS) analysis was performed on each wafer to better understand the increase in mobility as a function of wafer number. These data sets are included in the supplemental material $^{26}$ . In Fig. 2(d) we plot the concentration of oxygen atoms at the QW,  $N_{\rm o}$ , for each wafer. For wafers 1 to 11,  $N_{\rm o}$ decreases from  $8.7 \times 10^{18}/\text{cm}^3$  to the SIMS detection threshold of  $1 \times 10^{17}/\text{cm}^3$ . The steady decrease of oxygen content with increasing wafer number is likely due to reduced background in the reactor after the transfer of the wafers from the load lock to the growth chamber. The decrease in oxygen concentration is also correlated with the increase in mobility observed in Fig. 2(b-c). Wafer No. 26, which marks the beginning of a second cassette of wafers, shows an abrupt increase in  $N_{\rm o}$ , which is also correlated with a drop in the mobility. The combination of mobility and SIMS data suggest that oxygen contamination is a mobility limiting factor in these undoped Si/SiGe heterostructures. A similar correlation has been observed in undoped Si/SiGe heterostructures grown by molecular beam  $epitaxy^{27}$ .

In addition to the correlation between  $N_0$  and  $\mu$ , the data show that the heterostructure growth profile impacts the mobility of samples later in the growth series. As h is increased from 40 to 50 nm for Wafers No. 15 and 16, we observe a corresponding increase in  $\mu_{\rm H}$  and  $\mu_{\rm L}$ . For wafers 16–19, h is constant and both  $\mu_{\rm H}$  and  $\mu_{\rm L}$ show very little variation. At Wafer No. 20, h undergoes a large decrease from 50 to 20 nm, which is correlated with a large drop in mobility. For wafers 20-25, h increases from 20 to 50 nm and we see that the mobilities also recover to the values obtained from Wafer No. 19. In contrast, for lower wafer numbers, the correlations between h and mobility are weaker, suggesting that  $N_{\rm o}$  is the dominant mobility-limiting mechanism in these wafers. To obtain a better quantitative understanding of these correlations, we perform detailed measurements on Wafer No. 5 and 16 at T = 0.35 K in order to contrast the properties of a low and high mobility wafer.

# **IV. HIGH MOBILITY SAMPLE**

Based on its high 4.2 K mobility, a Hall bar from Wafer No. 16 was cooled down in a <sup>3</sup>He cryostat for further study. The oxygen content at the QW is  $N_{\rm o} = 5.0 \times 10^{17}/{\rm cm^{326}}$ . Figure 3 shows  $\rho_{\rm xx}$  and  $\rho_{\rm xy}$  as a function of *B* up to 8 T, with  $n = 2.17 \times 10^{11}/{\rm cm^2}$ . From the low field magnetotransport data we extract  $\mu = 1.62 \times 10^5 {\rm cm^2/Vs}$ . We observe quantum Hall plateaus in  $\rho_{\rm xy}$ 



FIG. 2: (a) SiGe spacer layer thickness, h, for wafers 1–26. Wafers with solid (hollow) symbols have a 2 nm (4 nm) thick Si cap. QW thicknesses are represented by symbol shapes. Circles: 5 nm, rectangles: 8 nm, triangles: 11 nm. (b)  $\mu_{\rm H}$  is the T = 4.2 K mobility at  $n_{\rm H} = 7 \times 10^{11}/{\rm cm}^2$ . (c)  $\mu_{\rm L}$  is the T = 4.2 K mobility at  $n_{\rm L} = 2.1 \times 10^{11}/{\rm cm}^2$ . (d)  $N_{\rm o}$  is the concentration of oxygen atoms inside the QW.

at consecutive integer filling factors  $\nu$  for B > 1.5 T, which indicates that both spin and valley degeneracies are lifted. In addition,  $\rho_{\rm xx}$  displays clear zeros, ruling out parallel conduction paths. For  $\nu > 6$ , plateaus in  $\rho_{\rm xy}$  are no longer visible, although oscillations in  $\rho_{\rm xx}$  are visible up to  $\nu = 24$ .

Figure 4 shows  $\mu$  as a function of n at five temperatures. At T = 0.35 K,  $\mu(n)$  is not well described by a single exponent, an often observed feature in 2DEG systems<sup>17</sup>. Our data differ from previous work<sup>23</sup>, where an exponent of  $\alpha = 1.7$  is observed in the density range of  $n = 0.6 - 4.5 \times 10^{11}$  /cm<sup>2</sup>. For  $n < 1 \times 10^{11}$ /cm<sup>2</sup>, the data roughly follow a  $\mu \propto n^{1.5}$  scaling, consistent with scattering due to remote charged impurities<sup>13</sup>. At higher  $n, \mu$  increases more slowly and nearly saturates when  $n > 5 \times 10^{11}$ /cm<sup>2</sup>. The high density saturation likely arises from impurity charges located very near or inside the QW, which lead to values of  $\mu$  that are only weakly dependent on  $n^{13}$ . It is notable that the mobility curves are temperature dependent at low densities, but all saturate to nearly the same high density value of 250,000 cm<sup>2</sup>/Vs. Another feature of the higher temperature data



FIG. 3: Wafer No. 16.  $\rho_{\rm xx}$  (red) and  $\rho_{\rm xy}$  (black) as a function of B, with  $V_{\rm G} = 0.75$  V and T = 0.35 K. We observe clear quantum Hall plateaus in  $\rho_{\rm xy}$  at integer filling factors  $\nu$  for B > 1.5 T.



FIG. 4: Wafer No. 16.  $\mu(n)$  for five different temperatures. The dashed lines show the predicted slopes for remote ionized impurity scattering and scattering due to impurities in the QW<sup>13</sup>. The charged impurity densities used to produce the two dashed lines are  $3.7 \times 10^{12}$ /cm<sup>2</sup> at a distance of 50 nm from the QW center (where the Al<sub>2</sub>O<sub>3</sub>/Si interface is) for remote impurity scattering, and  $3.4 \times 10^9$ /cm<sup>2</sup> in the QW center.

is that the density dependence of  $\mu(n)$  becomes stronger, though the curvature persists up to 4 K. At T = 4 K, the data approximately follow a  $\mu \propto n^{1.5}$  trend for  $n < 3 \times 10^{11}/\text{cm}^2$ .

To further probe the scattering mechanisms that limit the mobility of Wafer No. 16, we measure low-field SdH oscillations in the longitudinal resistivity,  $\rho_{xx}$ . We subtract the slowly varying background  $\rho_b$  from  $\rho_{xx}$  as outlined by Coleridge *et al.*<sup>18</sup> yielding  $\Delta \rho_{xx} = \rho_{xx} - \rho_b$ .  $\Delta \rho_{xx}$  is plotted against 1/B for three densities in Fig. 5(a). Clear periodic oscillations are observed, with a pe-



FIG. 5: Wafer No. 16. (a)  $\Delta \rho_{\rm xx}$  as a function of 1/B for three electron densities at T = 0.4 K. Traces have been offset by 150  $\Omega$  for clarity. (b) Dingle plots for the data in (a). Values of  $\Delta \rho_{\rm xx}$  used in this plot are the average of the maximum and minimum of each period of the SdH oscillations shown in (a). (c)  $\tau_{\rm q}$  and  $\tau_{\rm t}$  as functions of n at T = 0.4 K. (d) Dingle ratio  $\tau_{\rm t}/\tau_{\rm q}$  as a function of n at T = 0.4 K. The dashed line is a guide to the eye.

riodicity of 4 in  $\nu$ . This is consistent with the 2-fold spin degeneracy and 2-fold valley degeneracy at low fields. At higher fields B > 0.7 T, splitting of the peak in each period of the SdH oscillation becomes visible, due to increased Zeeman splitting. This splitting is examined in detail in Section VIII. We extract the amplitude of the oscillations in  $\Delta \rho_{\rm xx}$  at each period in  $1/B^{28}$  which is fit to:

$$\Delta \rho_{\rm xx} = 4\rho_0 X(T) \exp(-\pi/\omega_{\rm c}\tau_{\rm q}) \tag{1}$$

where  $\tau_{\rm q}$  is the quantum lifetime of the electrons,  $\rho_0$  is the zero-field resistivity,  $X(T) = (2\pi^2 k_{\rm B}T/\hbar\omega_{\rm c})/\sinh(2\pi^2 k_{\rm B}T/\hbar\omega_{\rm c})$  is the temperaturedamping factor,  $\omega_{\rm c} = eB/m^*$  is the cyclotron frequency, and  $k_B$  is the Boltzmann's constant. We use a constant effective mass  $m^* = 0.2m_{\rm e}$ , where  $m_{\rm e}$  is the free electron mass, for all fits<sup>29</sup>. Figure 5(b) shows the results of such fits, known as Dingle plots. The slopes of the Dingle plots<sup>19</sup> are inversely proportional to the quantum lifetime  $\tau_{\rm q}$  and imply shorter quantum lifetimes at lower densities.

In Fig. 5(c), we compare the transport lifetime,  $\tau_{\rm t}$ , and the quantum lifetime,  $\tau_{\rm q}$ , across the electron density range  $n = 1.8-6.8 \times 10^{11}/{\rm cm}^2$ . Values of  $\tau_{\rm t}$  are obtained<sup>30</sup> from the mobility data in Fig. 4 via  $\tau_{\rm t} = \mu m^*/e$  and values of  $\tau_{\rm q}$  are obtained from analysis of the low field SdH oscillations. Both lifetimes show similar de-



FIG. 6: Wafer No. 16. (a)  $\Delta \rho_{\rm xx}$  as a function of 1/B for  $n = 6.7 \times 10^{11}/{\rm cm}^2$  at four different temperatures. (b) Dingle plots for the data shown in (a). (c)  $\tau_{\rm q}$  and  $\tau_{\rm t}$  as a function of T at  $n = 6.7 \times 10^{11}/{\rm cm}^2$ . (d) Dingle ratio as a function of T. The dashed line is a guide to the eye.

pendencies on n and Dingle ratios, defined as  $\tau_{\rm t}/\tau_{\rm q}$ , range from 4 to 7 as shown in Fig. 5(d). In comparison with previous work on  $GaAs/AlGaAs^{19}$  and modulation-doped  $SiGe^{21}$  where the Dingle ratios typically range from 10 to 20, the Dingle ratios measured for this undoped sample are sizably smaller, indicating that large angle scattering plays a more dominant role in this sample. Such a situation would arise when the distribution of impurities is more concentrated towards the location of the  $2\text{DEG}^{13}$ . This is unexpected in an undoped system where charged impurities are thought to reside mostly in the  $Al_2O_3/Si$ interface<sup>23</sup>,  $\sim 50$  nm away from the 2DEG in this sample. Our interpretation of the possible cause for such distribution is the peak in oxygen impurities at the 2DEG location<sup>26</sup>. Ionization of a small fraction of these oxygen atoms would lead to a sizable amount of impurity charges inside the QW, which contribute to large angle scattering with a Dingle ratio near unity. The decreasing trend of the Dingle ratio at higher densities also differs from theoretical calculations based on a single dopant sheet  $^{15}$ . This deviation is interpreted to be due to the mitigated contribution of remote impurity scattering to the overall momentum scattering rate at higher densities, since the scattering rate  $\tau_t^{-1} \propto n^{-1.5}$  for remote impurities but  $\tau_t^{-1} \propto n^{-0.1}$  for impurities inside the QW. At higher densities, scattering from impurities inside the QW becomes more dominant than remote impurities, which reduces the overall Dingle ratio.

The quantum lifetime  $\tau_q$  for this high mobility sam-

ple is also measured as a function of T at  $n = 6.7 \times 10^{11}/\text{cm}^2$ . Figure 6(a–b) displays low field SdH oscillations and the associated Dingle plots. The extracted values of  $\tau_q$  are plotted alongside  $\tau_t$ , obtained by measuring the temperature-dependent mobility at this density [Fig. 6(c)]. The transport lifetime is relatively insensitive to temperature, while the quantum lifetime varies by nearly a factor of 4 from T = 0.4 K to 1.5 K. The resulting Dingle ratio, plotted in Fig. 6(d), increases almost linearly with temperature from 4 to 11. These data are in contrast with a single-particle description of electron scattering in 2DEGs<sup>14,15,31</sup>, where the temperature dependence of both lifetimes is expected to be weak in the  $T \ll T_{\rm F}$  regime, where  $T_{\rm F}$  is the Fermi temperature (approximately 47 K at this density).

Arapov et al.<sup>32</sup> have recently measured an In-GaA/GaAs double QW structure and report a similar, strong temperature dependence of  $\tau_{\rm q}$  at  $T \ll T_{\rm F}$ , which the authors attribute to electron-electron interactions. A similar mechanism may explain the trends observed in this work. While electron-electron interactions may be significant, our analysis is based on the established single-particle model due to the fact that electron-electron interactions are expected to renormalize both  $\tau_{\rm q}$  and  $m^{*33,34}$ . The observed temperature dependence of  $\tau_{\rm q}$  in Fig. 6(c) could be due to a change in  $\tau_{\rm q}$  with temperature or an apparent change in  $\tau_{\rm q}$  due to a renormalize  $m^*$ . It is difficult to distinguish between these two possibilities based on the SdH data alone.

#### V. LOW MOBILITY SAMPLE

We next examine data from Wafer No. 5, which has a much lower maximum mobility of  $\mu = 7.5 \times 10^4 \text{ cm}^2/\text{Vs}$ at 4.2 K. Wafer No. 5 has a 2 nm thick Si cap, a h = 40 nm thick SiGe spacer layer, and a 5 nm wide Si QW. SIMS analysis shows a similar distribution of oxygen inside the SiGe spacer as the high mobility sample<sup>26</sup>. However, the oxygen content in the QW is peaked at  $N_o = 2.5 \times 10^{18}/\text{cm}^3$ , which is five times higher than the high mobility sample.

Figure 7 shows the results of magnetotransport measurements on this low mobility sample.  $\mu(n)$  is plotted in Fig. 7(a) and increases with n, although with a weaker dependence than the high mobility sample.  $\mu(n)$ is also temperature dependent, and more strongly scales with n at higher temperatures. At T = 0.35 K,  $\mu(n)$ is nearly density-independent. As T increases,  $\mu(n)$  becomes more density-dependent and eventually reaches an approximate scaling of  $\mu \propto n^{0.7}$  at T = 4 K. The smaller power-law exponent for this sample suggests that remote impurity scattering plays a less significant role compared to the high mobility sample. Instead, electron scattering is likely dominated by impurity charges situated inside the QW, which is consistent with the higher oxygen content observed in the SIMS data<sup>26</sup>.

Figure 7(b) shows  $\tau_{q}$  and  $\tau_{t}$  for the low mobility sam-



FIG. 7: Wafer No. 5 (low mobility sample). (a)  $\mu(n)$  at five different temperatures. The dashed line shows the prediction for scattering from impurities in the QW with a charged impurity density of  $1.3 \times 10^{10}/\text{cm}^2$  at the QW center. (b)  $\tau_{\rm q}$ and  $\tau_{\rm t}$  plotted as a function of n, extracted from low field SdH oscillations. T = 0.4 K in this plot. (c) Dingle ratios  $\tau_{\rm t}/\tau_{\rm q}$  obtained from the data in (b).

ple at five different densities and with T = 0.4 K. Both lifetimes are shorter at lower electron densities, similar to the high mobility sample. Despite the factor of  $\sim 3$  difference in  $\tau_{\rm t}$  between the two samples, the values of  $\tau_{\rm q}$  are very similar. This observation agrees well with recent theoretical results by Das Sarma et al.<sup>35</sup>, who considered a two-impurity model and showed that increasing (decreasing)  $\tau_{\rm t}$  does not necessarily lead to increasing (decreasing)  $\tau_{\rm q}$  when there is more than one scattering mechanism. We also plot the density-dependent Dingle ratio  $\tau_t/\tau_q$  of this sample in Fig. 7(c).  $\tau_t/\tau_q$  ranges from 1.3 at high density to 2.3 at low density, significantly smaller than the high mobility sample. The smaller Dingle ratio observed in this sample implies that the underlying scattering events are even larger in angle compared to the high mobility sample, consistent with scattering from QW impurities.

## VI. ESTIMATE OF DEFECT DENSITIES

Monroe *et al.* have carefully analyzed seven scattering mechanisms that are potentially relevant to the Si/SiGe materials system<sup>13</sup>. Among these mechanisms, alloy scattering, scattering due to strain modulation, scattering due to vicinal surfaces and scattering from threading dislocations are estimated to limit mobilities to above  $10^7$  $\rm cm^2/Vs$ , two orders of magnitude higher than the mobilities measured in our samples. Interface roughness has been reported to be an important factor in a  $\sim 500$  nm deep Si/SiGe QW structure<sup>24</sup>, but is expected to lead to a mobility that decreases with increasing density (a trend that is not observed in our data). We therefore limit our analysis to the two remaining scattering mechanisms: remote impurity scattering from charges located at the Al<sub>2</sub>O<sub>3</sub>/Si interface and scattering from oxygen related background charges in the QW.

We now compare the experimental data with these predictions, starting with the high mobility sample. Figure 4 shows  $\mu(n)$  for Wafer No. 16. At low densities,  $\mu(n)$ roughly follows the  $\mu \propto n^{1.5}$  power law expected for remote impurity scattering, while for higher densities  $\mu$  is a weak function of n. Superimposed on the data are dashed lines showing the expected scaling for remote impurity scattering and scattering from impurities in the QW calculated using theoretical results of Monroe *et al.* We set the distance between the remote impurities and the 2DEG to be h = 50 nm such that the remote impurities are Al<sub>2</sub>O<sub>3</sub>/Si interface charges, as reported by Li et al.<sup>23</sup>. The 2D remote impurity density is adjusted to  $n_1 = 3.7 \times 10^{12} / \text{cm}^2$  to bring theory into agreement with the data. Similarly, for scattering from impurities in the QW we find reasonable agreement with the data when the 2D QW impurity density  $n_2 = 3.4 \times 10^9 / \text{cm}^2$ . Dingle ratio data for Wafer No. 16 are plotted in Fig. 5(d) and show a linear decrease with n over the entire density range. This is broadly consistent with a crossover from remote impurity scattering limited transport to local defect scattering-limited transport as n increases.

In comparison,  $\mu(n)$  is shown for the low mobility sample (Wafer No. 5) in Fig. 7(a). At T = 0.35 K, the mobility is weakly dependent on density over the entire density range, consistent with scattering from impurities in the QW. The dashed line shows the prediction for scattering from impurities in the QW taking  $n_2 = 1.3 \times 10^{10}/\text{cm}^2$ . We note that this defect density is 4 times higher than the high mobility sample, reminiscent of the factor of 5 difference between the oxygen contents in the QWs of the low and high mobility samples<sup>26</sup>. It is also clear that the Dingle ratio is much less sensitive to density, with  $\tau_t/\tau_q \sim 1-2$  over the entire density range. The small Dingle ratio is consistent with scattering from impurities in the QW.



FIG. 8: Wafer No. 16.  $\rho_{\rm xx}(T)$  at B = 0 T for n = 0.34, 0.36, 0.38, 0.40, 0.42, 0.46, 0.51, 0.59, 0.73 and 0.96  $\times 10^{11}/{\rm cm}^2$  (from top to bottom). A metal-insulator transition occurs at  $n_{\rm c} = 0.46 \times 10^{11}/{\rm cm}^2$ .

## VII. METAL-TO-INSULATOR TRANSITION

For spin-based quantum information processing, quantum dots are typically operated in the few-electron regime<sup>12</sup>. One important gauge for the degree of disorder at low electron density is the critical electron density,  $n_c$ , for the metal-to-insulator transition (MIT) in 2DEGs. For silicon, a MIT has been observed in MOSFETs<sup>36,37</sup>, modulation doped Si/SiGe structures<sup>38–40</sup>, an undoped Si/SiGe 2DEG structure<sup>41</sup>, and an ambipolar Si-vacuum FET<sup>42</sup>. Values of  $n_c$  vary greatly in Si/SiGe systems, ranging from 0.32 to  $4.05 \times 10^{11}$ /cm<sup>238–41</sup>.

The experimental signature for the MIT in 2DEG systems is a sign reversal in  $d\rho/dT$ , where  $\rho$  is the resistivity of the system<sup>36</sup>. For  $n > n_c$ ,  $d\rho/dT > 0$  and the 2DEG displays metallic behavior. For  $n < n_c$ ,  $d\rho/dT < 0$  and the 2DEG behaves as an insulator. In Fig. 8, we plot  $\rho_{\rm xx}(T)$  for the high mobility sample at ten different densities below  $n = 1.0 \times 10^{11}/{\rm cm}^2$ . We observe the following features in this data set:

1. At the lowest two densities  $n = 0.34 \times 10^{11} / \text{cm}^2$  and  $0.36 \times 10^{11} / \text{cm}^2$ ,  $d\rho_{\text{xx}}/dT < 0$  throughout the measured temperature range. In addition,  $\rho_{\text{xx}}$  appears to diverge exponentially at T < 1 K, indicative of a true insulating phase<sup>43</sup>.

2. At the next three higher densities n = 0.38, 0.40 and  $0.42 \times 10^{11}$ /cm<sup>2</sup>,  $\rho_{\rm xx}$  varies non-monotonically with temperature. While  $d\rho_{\rm xx}/dT < 0$  at T = 4.2 K,  $d\rho_{\rm xx}/dT > 0$  for a small, intermediate temperature range. We note that this behavior has also been observed by Lu *et al.* in another undoped Si/SiGe sample<sup>41</sup>, and is common in Si MOSFET systems<sup>44</sup>.

3.  $d\rho_{\rm xx}/dT>0$  at 0.5 K for  $n\geq n_{\rm c},$  where  $n_{\rm c}=0.46\times 10^{11}/{\rm cm}^2.$ 

4. At  $n \ge n_{\rm c}$ , with the exception of  $n = 0.51 \times 10^{11}$ 

 $/\text{cm}^2$ ,  $d\rho_{\text{xx}}/dT > 0$  up to a crossover temperature  $T_{\text{c}}$ . For  $T > T_{\text{c}}$ ,  $d\rho_{\text{xx}}/dT < 0$ . Furthermore,  $T_{\text{c}}$  increases with increasing *n*. Das Sarma *et al.* interpreted this behavior as a quantum-to-classical crossover<sup>14,43,45</sup>.

We note that the critical density is comparable to the lowest value of  $0.32 \times 10^{11}/\text{cm}^2$  that has been reported in doped Si/SiGe structures<sup>40</sup>, and a factor of 4 lower than the value of  $1.9 \times 10^{11}/\text{cm}^2$  observed in a previous work on undoped Si/SiGe structure<sup>41</sup>, indicating a very low level of disorder in our undoped sample. The critical density observed in our system lies at the lower end of the critical density spectrum<sup>46</sup> and within an order of magnitude of the lowest value of  $n_c = 7.7 \times 10^9/\text{cm}^2$  in a GaAs system<sup>47</sup>. We have successfully measured fewelectron charge stability diagrams for quantum dots fabricated from Wafer No.  $16^{48}$ , which gives further evidence of a low disorder potential.

# VIII. VALLEY SPLITTING

Another important figure of merit for the Si/SiGe quantum well system is the valley splitting. Measurements of the valley splitting in Si MOSFET systems have been extensively performed. Most values range from  $0.7 - 1.5 \text{ meV}^{49,50}$ , with one study reporting a value as large as 23 meV<sup>51</sup>. In comparison, the valley splitting in Si/SiGe systems tends to be smaller, ranging from  $0.05 - 0.3 \text{ meV}^{52-54}$ . In this section, we determine  $\Delta_{v}$  through careful analysis of the SdH oscillations in Wafer No. 16.

In Fig. 9 we plot  $\rho_{\rm xx}(B)$  with  $n = 6.6 \times 10^{11}/{\rm cm}^2$ . SdH oscillations are observed above an effective field  $B_{\rm eff}$ = 0.38 T and have a periodicity of 4 in  $\nu$ . For  $B > B_{\rm s} =$ 0.88 T, we observe change in periodicity of the SdH oscillations, indicating that spin degeneracy has been lifted. The periodicity changes again beyond  $B_{\rm v} = 1.8$  T, consistent with the lifting of both spin and valley degeneracies. We have verified that the spin degeneracy is lifted before valley degeneracy using the tilted field method<sup>52,53</sup>.

The energy spectrum of 2D electrons in a perpendicular field is described by four characteristic energy scales. The first is the Zeeman splitting,  $E_z = g\mu_B B$ , where  $\mu_B$ is the Bohr magneton and g is the electronic g-factor. The second is  $E_{\rm l} = e\hbar B/m^* - E_{\rm z}$ , which is the Landau level spacing minus the Zeeman splitting. The third is the valley splitting,  $\Delta_{\rm v}$ . Finally, clear SdH oscillations will only be observed when the Landau level spacing is greater than the Landau level broadening  $\Gamma \approx \hbar/2\tau_a$ . Spin splitting becomes visible when  $E_{\rm z}(B_{\rm s}) \approx \Gamma$ . Based on the effective field at which the SdH oscillations become visible, we estimate  $\Gamma \approx E_{\rm l}(B_{\rm eff})$ . We then have the relation  $E_z(B_s) \approx E_l(B_{eff})$ , allowing us to extract  $g = 3.0 \pm 0.2$ . The g-factor is in reasonable agreement with the value of  $g = 2.9 \pm 0.1$  at  $n = 5.9 \times 10^{11}$  /cm<sup>2</sup> found in a previous study<sup>53</sup>. Based on this experimental value of g, we find  $\Gamma \sim 150 \pm 10 \mu \text{eV}$ . Finally, the valley degeneracy is lifted at the field for which  $\Delta_{\rm v}(B=1.8~{\rm T})$  $\sim 150 \ \mu eV$ . The valley splitting is substantial and com-



FIG. 9: Wafer No. 16.  $\rho_{\rm xx}(B)$  at T = 0.4 K. SdH oscillations are observed beyond  $B_{\rm eff} = 0.38$  T. Spin (valley) degeneracy is lifted at  $B_{\rm s} = 0.88$  T ( $B_{\rm v} = 1.8$  T).

parable to the two-electron singlet-triplet splitting that is measured in GaAs quantum  $dots^{3,4}$ .

# IX. CONCLUSIONS

We have measured 26 wafers with different growth parameters to identify the dominant mobility limiting mechanisms in undoped Si/SiGe QW heterostructures. At 4.2 K we find correlations between mobility and oxygen content at the QW as well as the thickness of the top SiGe spacer. We also measured  $\tau_{\rm t}$  and  $\tau_{\rm q}$  for two Si/SiGe QW heterostructures across a wide density range at  $T \sim$ 0.35 K. Based on the density dependencies of the two lifetimes, we conclude that the mobility of high quality samples with low oxygen content at the QW is mostly limited by remote impurity charges, while the lower mobility samples with high oxygen content in the QW are limited by the impurity charges inside or very close to the QW, consistent with the correlations observed at 4.2 K. To further assess the merits of the high mobility heterostructure as a platform for spin-based quantum dots, we have measured a low critical density  $n_{\rm c} = 0.46 \times 10^{11}$  $\rm cm^2$  for the MIT and a valley splitting  $\Delta_v \sim 150 \ \mu eV$ .

While we cannot rule out effects due to other impurities, our SIMS results suggest that significant improvements in the electron mobility may be obtained by reducing the level of oxygen content in the Si/SiGe heterostructure. Our data give no information about the microscopic scattering mechanism that results from the oxygen impurities. The literature suggests several possibilities: a) lattice strain due to interstitial and substitutional oxygen<sup>55</sup>, b) thermal donor generation<sup>56</sup>, and c) enhanced donor generation rate due to the presence of carbon impurities<sup>57</sup>. Further work is needed to identify the mechanism that leads to the correlation between oxygen concentration and mobility.

The SiGe spacer layer thickness can also be increased to reduce scattering from charged impurities at the surface of the wafer. This second approach has limitations for quantum dot devices, as it is desirable to have strong in-plane electrostatic confinement, which is harder to obtain in samples with deeper QWs. The magnetic fields at which the valley splitting was extracted corresponds to a cyclotron radius of  $\sim 20$  nm, which is a realistic size for the lithographic patterning of quantum dots on Si. Therefore efforts should also be directed towards reducing the size of Si quantum dots to emulate high levels of magnetic confinement, which yielded large values of val-

- \* Present Address: Department of Physics, Harvard University, Cambridge, MA 02138, USA
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ley splitting in this work. Overlapping gate architectures may prove helpful to achieve tight electronic confinement in the relatively high effective mass Si/SiGe quantum well system<sup>48</sup>.

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