Quantum Transport Properties of Industrial $^{28}$Si/$^{28}$SiO$_2$

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We investigate the structural and quantum transport properties of isotopically enriched $^{28}$Si/$^{28}$SiO$_2$ stacks deposited on 300-mm Si wafers in an industrial CMOS fab. Highly uniform films are obtained with an isotopic purity greater than 99.92%. Hall-bar transistors with an oxide stack comprising 10 nm of $^{28}$SiO$_2$ and 17 nm of Al$_2$O$_3$ (equivalent oxide thickness of 17 nm) are fabricated in an academic cleanroom. A critical density for conduction of $1.75 \times 10^{11}$ cm$^{-2}$ and a peak mobility of 9800 cm$^2$/Vs are measured at a temperature of 1.7 K. The $^{28}$Si/$^{28}$SiO$_2$ interface is characterized by a roughness of $\Delta_1 = 0.4$ nm and a correlation length of $\Lambda_1 = 3.4$ nm. An upper bound for valley splitting energy of 480 $\mu$eV is estimated at an effective electric field of 9.5 MV/m. These results support the use of wafer-scale $^{28}$Si/$^{28}$SiO$_2$ as a promising material platform to manufacture industrial spin qubits.

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I. INTRODUCTION

Enrichment of the spin-zero $^{28}$Si isotope drastically reduces spin-bath decoherence in silicon [1,2] and has enabled solid-state spin qubits with extremely long coherence [3,4] and high control fidelity [5–7]. The limited availability of isotopically enriched $^{28}$Si in industrially adopted forms [8], however, was previously thought to be a major bottleneck to leverage CMOS technology for manufacturing qubits with the quality and in the large numbers required for fault-tolerant quantum computation [9,10]. Recently, isotopically enriched silane ($^{28}$SiH$_4$) has been employed in a preindustrial CMOS facility to deposit high-quality $^{28}$Si epiwafers [11]. Crucially, an industrial supply of $^{28}$SiH$_4$ has been established and silicon quantum dots were fabricated on a wafer-scale $^{28}$Si/$^{28}$SiO$_2$ stack grown in an industrial manufacturing CMOS fab [12]. In these quantum dots, a single-electron spin lifetime of 2.8 ms was obtained at a temperature of 1.1 K and weak charge noise was measured, pointing to a promising material platform for qubit operation at elevated temperatures.

Studies devoted to $^{28}$Si quantum dots, however, tend to discuss only marginally the structural properties of the originating $^{28}$Si/$^{28}$SiO$_2$ material stack and the electrical transport in the associated 2DEG. In this paper we provide structural characterization of the same industrial $^{28}$Si wafer used for quantum dots in Ref. [12] and assess the disorder properties of the critical $^{28}$Si/$^{28}$SiO$_2$ interface. By investigating the quantum transport properties of Hall-bar transistors, we extract key material metrics such as carrier mobility, critical density, interface roughness, interface correlation length, and valley splitting energy. Electron mobility is typically used as a figure of merit to assess the quality of the semiconductor-oxide interface. However, peak mobility is measured at high electron density, where screening effects are relevant [13,14]. The critical density, instead, indicates the minimum density required to establish metallic conduction by overcoming electron trapping at the oxide interface. As such, the critical density is a complementary metric to the mobility and characterizes the interface disorder at low densities, where quantum devices typically operate. Overall, large mobility and small critical density indicate material uniformity and low disorder at the confining interfaces. These properties are beneficial for obtaining reproducible quantum dots at intended locations on the substrate. Valley splitting quantifies the energetic separation between the ground state used for computation and the lowest excited state. A sharp flat interface is required to achieve large splitting energy, which is beneficial for qubit operation [15,16]. The results reported
in this work indicate a low disorder environment at the $^{28}$Si/$^{28}$SiO$_2$ interface and potential to achieve large valley splitting, supporting the industrial integration of spin qubits on wafer-scale $^{28}$Si.

II. MATERIAL CHARACTERIZATION

The schematics in Fig. 1 illustrate the key steps in the supply chain of isotopically enriched precursors for wafer-scale epitaxial growth of $^{28}$Si. A silicon-tetrafluoride gas (SiF$_4$) with natural abundance of $^{28}$Si of 92.23% is isotopically enriched in $^{28}$Si to a concentration greater than 99.92% by centrifuge separation. The $^{28}$SiF$_4$, with a residual $^{29}$Si concentration of 0.08%, is then reduced to obtain high purity $^{28}$SiH$_4$. $^{28}$SiH$_4$ gas cylinders (1% dilution in H$_2$) have been installed for use in a state-of-the-art chemical-vapor deposition tool of a 300-mm fabrication line to deposit $^{28}$Si epilayers. Maintaining the chemical purity of gas precursors throughout the supply chain is crucial to obtain a low disorder $^{28}$Si/$^{28}$SiO$_2$ stack. The growth process starts with the deposition of 1 $\mu$m of intrinsic natural Si on a high-resistivity 300-mm Si(100) wafer followed by a 100-nm-thick intrinsic $^{28}$Si epilayer. The wafer is then thermally processed at high temperature for the formation of a high-quality 10-nm-thick $^{28}$SiO$_2$ layer. The oxidation process is based on prior Intel transistor technology [17–19]. In this work, the allowed thermal budget for oxidation is optimized [20] to minimize Si self-diffusion and obtain sharp isotopic profiles, as evident in the secondary ion mass spectroscopy profiles in Fig. 1.

In Fig. 1 we compare morphology and composition of the grown stack at the center and the edge of the 300-mm wafer. No difference in surface or interface roughness, composition, and purity can be observed across the wafer, indicating a uniform film deposition. Atomic force microscopy shows a uniform and near defect-free surface with a root-mean-square surface roughness of 0.2 nm measured over an area of 1 $\mu$m x 1 $\mu$m. Secondary ion mass spectroscopy of isotopes $^{28}$Si, $^{29}$Si, and $^{30}$Si shows a high-purity film with a residual concentration of nonzero-spin nuclei $^{29}$Si reduced from 4.76% in the Si buffer to 0.08% in the purified epilayer, demonstrating that the precursor purity is preserved during the deposition process. The concentration of common background contaminants C and O is below the detection limit of 4 $\times$ 10$^{17}$ cm$^{-3}$ and 1 $\times$ 10$^{18}$ cm$^{-3}$, respectively. Background doping from P and B is also below the detection limit of 3 $\times$ 10$^{15}$ cm$^{-3}$ and 1 $\times$ 10$^{14}$ cm$^{-3}$, respectively. High-resolution transmission electron microscopy shows that no dislocations or stacking faults are visible in the epilayer. Moreover, the $^{28}$Si/$^{28}$SiO$_2$ interface is flat down to one–two atomic layers over distances ($\approx$200 nm) that are larger than the

![Diagram of material characterization](image-url)
quantum-dot spin qubits (≤50 nm). This increases the chance of defining a quantum dot in a step-free area, which is beneficial for obtaining large valley splitting [15,16]. The sharpness of the interface, the negligible density of defects in the lattice, and the associated electron diffraction pattern highlight the film quality and the good control over the growth process despite the introduction of a new Si precursor in the manufacturing CMOS fab.

III. DEVICE FABRICATION AND TRANSPORT PROPERTIES

Moving on to device fabrication, Fig. 2(a) shows schematics and optical micrograph of a MOS transistor

![Schematic of MOS transistor](image)

(a) Schematics of the Hall-bar device fabrication, starting from the 300-mm $^{28}$SiO$_2$/2$^{28}$Si/Si(100) stack followed by coupon-sized processing. The optical micrograph of the final device shows the multiterminal geometry used for Hall measurements. (b) Source-drain current $I_{SD}$ measured as a function of top gate voltage $V_g$ at $T = 1.7$ K. (c) Linear relationship between 2DEG Hall density $n$ and top gate voltage $V_g$. (d) Channel mobility $\mu$ measured as a function of $n$ (black) and corresponding calculation (red) including scattering from charged impurities and from interface roughness. (e) 2DEG conductivity in the low density range (black) and fit to percolation theory (red).

The electrical characterization of the device is performed at a temperature of 1.7 K using standard four-terminal low-frequency lock-in techniques with a constant source-drain excitation voltage of 1 mV. Longitudinal ($\rho_{xx}$) and transverse ($R_{xy}$) resistivity are measured as a function of carrier density—controlled by the top gate—and external perpendicular magnetic field $B$. The Hall carrier density $n$ and the electron mobility $\mu$ are calculated using the relationships $R_{xy} = (ne)^{-1}B$ and $\mu = (ne\rho_0)^{-1}$, respectively, where $e$ is the elementary charge and $\rho_0 = \rho_{xx}(B = 0)$.

A dc voltage applied to the top gate ($V_g$) accumulates a 2DEG at the $^{28}$Si/$^{28}$SiO$_2$ interface, which conducts above a turn-on voltage of $V_{TO} = 1.22$ V [22], as shown in Fig. 2(b). For values below $V_{TO}$ no current flow is observed in the device up to a temperature of $T = 23$ K, confirming the insulating behavior of the intrinsic $^{28}$Si film at low temperature. For $V_g > V_{TO}$ [Fig. 2(c)] we measure a linear increase in the Hall density $n$ as a function of $V_g$. The experimental capacitance $C = e \, dn/dV_g = 0.19 \, \mu$F/cm$^2$ matches within 5% of the expected value for the given dielectric stack. Upon multiple sweeps of $V_g$ no hysteresis is observed and the same values of $V_{TO}$ and $C$ are measured, indicating a stable potential landscape at the oxide interface.

The experimental and theoretically calculated density-dependent mobility curves are shown in Fig. 2(d). Above a critical density, required to establish metallic conduction in the 2DEG, the mobility rises sharply due to screening from charged impurity Coulomb scattering [23–26]. A peak mobility of 9800 cm$^2$/Vs is reached at $n = 1.13 \times 10^{12}$ cm$^{-2}$, corresponding to a mean free path of 120 nm. Beyond, the mobility drops due to surface-roughness scattering at the $^{28}$Si/$^{28}$SiO$_2$ interface [23,25,26]. The calculated scattering-limited mobility takes into account a scattering charge density at the semiconductor-oxide
interface and an exponential autocorrelation function form of the interface roughness [13,25,26]. A good match is obtained for a scattering charge density of $4.65 \times 10^{10}$ cm$^{-2}$, an interface roughness of $\Delta = 0.4$ nm, and an interface correlation length of $\Lambda = 3.4$ nm (see Appendix). $\Delta$ describes the interface root-mean-square height fluctuations, $\Lambda$ is the lateral distance over which the fluctuations are correlated. The interface roughness is compatible with the morphology investigation by transmission electron microscopy reported in Fig. 1.

The critical density is extracted from a percolation fit of the density-dependent conductivity [Fig. 2(e)] $\sigma_{xx} \sim (n - n_p)^p$ [13,14], where $n_p$, $p$ are the percolation transition density and exponent, respectively. By fixing $p = 1.31$, as expected in a two-dimensional system, we estimate $n_p = 1.75 \pm 0.02 \times 10^{11}$ cm$^{-2}$ at $T = 1.7$ K. The fit used to estimate $n_p$ is performed over the density range $2.0 - 7.3 \times 10^{11}$ cm$^{-2}$ (see Appendix). Previous studies have shown that $n_p$ decreases with decreasing temperature [13,14], therefore the obtained value of $1.75 \times 10^{11}$ cm$^{-2}$ sets an upper bound for the critical density in the temperature regime at which qubits are typically operated ($T \leq 100$ mK).

Both the mobility and critical density obtained in the wafer-scale isotopically enriched $^{28}$Si/$^{28}$SiO$_2$ stack are qualitatively comparable to the values previously reported for high-mobility Si MOSFETs at low temperatures [13,14,21,27,28,30,31] (see Table I). In drawing a meaningful comparison with the data reported in the literature, the reader should consider material stacks that have produced quantum-dot devices using a similar process flow. For example, peak mobility is known to be higher in devices with thicker oxide [23,32] and degrades upon device exposure to e-beam [14,21].

Transport characterization at high magnetic field (Fig. 3) allows the measurement of effective mass $m^*$ and quantum lifetime $\tau_q$, from which we estimate an upper bound for the valley splitting energy and the $g$ factor. In Fig. 3(a) we report the longitudinal magnetoresistivity at a density $n = 1.05 \times 10^{12}$ cm$^{-2}$, which corresponds to an effective electric field of 9.5 MV/m. Shubnikov-de Haas (SdH) oscillations are observed, with minima aligned to quantum Hall plateaus in $R_{xy}$. SdH oscillations start at $B_{eff} = 1$ T and spin degeneracy is resolved at $B_S = 4.3$ T, corresponding to the even filling factor $\nu = 10$. Figure 3(b) shows the filling factor progression against $1/B$. High mobility and density allow filling factors to be resolved up to $\nu = 36$, with fourfold periodicity at low magnetic field due to spin and valley degeneracy and twofold periodicity beyond $B_S$. We do not observe odd filling factors, indicating that the twofold valley degeneracy is not resolved under these measurement conditions. From the linear filling factor progression we extract a density $n_{SdH} = 1.06 \times 10^{12}$ cm$^{-2}$. The agreement between the Hall density $n$ and $n_{SdH}$ indicates that only one high-mobility subband contributes to electrical transport, confirming the high-quality $^{28}$Si epitaxy.

The transverse effective mass $m^*$ of the high-mobility carriers is calculated from the damping of the SdH oscillations with increasing temperature, described by the relation [33–36]

$$\frac{\Delta \rho_{xx}(T, B)}{\Delta \rho_{xx}(T_0, B)} = \frac{T \sinh \chi}{T_0 \sinh \chi},$$

where $\Delta \rho_{xx}$ is the SdH oscillation amplitude after polynomial background subtraction, $\chi = 2\pi^2 k_B T / \hbar \omega_c$, $\chi_0 = \chi(T_0=1.7 \text{ K})$, $\omega_c = eB/m^*$ is the cyclotron frequency, $h$ is the Planck constant, and $k_B$ the Boltzmann constant. Figure 3(d) shows the temperature dependence of the oscillation amplitude at $B = 3.18$ T, before spin splitting, normalized to the amplitude at $T_0 = 1.7$ K. By fitting the data to Eq. (1) we obtain an effective mass of $m^* = 0.19m_e$.
between the filling factors and Zeeman spin splitting are resolved. (b) Linear relationship Arrows indicate the magnetic field at which SdH oscillations are dominant since most sources of scattering are located near the semiconductor-oxide interface. This result confirms the validity of the model used for the theoretically calculated mobility curve of Fig. 2(d) and suggests that scattering associated with the Al2O3 deposition is minimal, which is beneficial for quantum-dot fabrication.

From the obtained $\tau_q$ we calculate a Landau-level broadening of $\Gamma \approx \hbar/2\tau_q = 480 \mu eV$, which sets an upper bound to valley splitting at the investigated density (electric field) and magnetic field. For comparison, a valley splitting energy of 275 $\mu$eV is measured in $^{28}$Si quantum dots fabricated on the same wafer in an academic environment [12] and a valley splitting of 200 $\mu$eV is reported for electric fields of 10 MV/m in other quantum dots [38]. The electron $g$ factor is evaluated by considering that the onset of spin splitting at $B_S$ implies a Zeeman energy $g\mu_B B_S \approx \Gamma$, where $\mu_B$ is the Bohr magneton. From this, a $g$ factor of $g = 1.92 \pm 0.07$ is estimated, which is close to the expected single-particle value of $g = 2$.

### IV. CONCLUSION

In conclusion, we investigate the structural and quantum transport properties of isotopically enriched $^{28}$Si/$^{28}$SiO$_2$ stacks deposited on 300-mm wafers in an industrial CMOS fab. The material characterization shows that the level of control achieved in the growth process results in a uniform deposition with high-purity epilayers and a sharp semiconductor-oxide interface. Detailed quantum transport characterization of Hall-bar devices fabricated in an academic cleanroom points to a high-quality $^{28}$Si/$^{28}$SiO$_2$ interface, promising for hosting spin qubits. Mobility and critical density for these stacks are among the best reported for gate stacks used for quantum-dot fabrication, with the potential to achieve large valley splitting. Disorder at the critical semiconductor-oxide interface is expected to further decrease by processing the entire gate stack in the high-volume manufacturing environment, because an advanced process control is attainable and e-beam-induced damage is avoided.

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### APPENDIX: THEORETICAL CALCULATIONS AND FITTING PROCEDURES

#### 1. Mobility-density curve

To assess how sensitive the calculated mobility curve is to the input parameters (i.e., interface roughness $\Delta$, interface correlation length $\Lambda$, and scattering charge density $n_s$), in Fig. 4 we show the mobility curve calculated by varying the parameters one at a time, starting from the best values that generated the theoretical curve reported in Fig. 2(d).

The theoretical curve is more sensitive to variations in $\Delta$ and $n_s$, compared to $\Lambda$. In fact, a variation of 5% in $\Delta$...
or \( n_i \) results in a maximum variation in the mobility up to approximately 10% and approximately 5%, respectively. A variation of 5% in \( \Lambda \) results, instead, in a negligible variation in the mobility (0.1%). We note that variations of 5% in \( n_p \) for smaller density ranges, the extracted value of \( n_p \) shows a weak dependency on the density range used for the fit, with all the values between 1.70 \( \times 10^{11} \) cm\(^{-2} \) and 1.75 \( \times 10^{11} \) cm\(^{-2} \). The chosen value of \( n_p = 1.75 \times 10^{11} \) cm\(^{-2} \) is therefore a valid estimate since it is extracted considering a significant density range and further extending this range does not result in improvements in the error intervals.

![Graph showing extracted percolation density \( n_p \) as a function of the density range \( \Delta n \) over which the fit is performed. The lower bound of all the density ranges is \( n = 2.0 \times 10^{11} \) cm\(^{-2} \). The widest range considered here includes a maximum density of \( n = 1.08 \times 10^{12} \) cm\(^{-2} \), close to the value at peak mobility of \( n = 1.13 \times 10^{12} \) cm\(^{-2} \). The point in red corresponds to a fit result of \( n_p = 1.75 \pm 0.02 \times 10^{11} \) cm\(^{-2} \).](image)

2. Percolation transition density

The percolation theory considered to evaluate the percolation transition density \( n_p \) is valid only in a density range \( \Delta n \) close to \( n_p \) and for \( n > n_p \). For this reason, the fit reported in Fig. 2(e) of the main text is performed considering a density range of 2.0–7.3 \( \times 10^{11} \) cm\(^{-2} \), resulting in \( n_p = 1.75 \pm 0.02 \times 10^{11} \) cm\(^{-2} \).

To clarify how the density range is chosen to fit the data, in Fig. 5 we show \( n_p \) as a function of the range over which the fit is performed. The density range \( \Delta n \) is increased by fixing the lowest density at 2.0 \( \times 10^{11} \) cm\(^{-2} \) and increasing the highest density value. While the error intervals increase for smaller density ranges, the extracted value of \( n_p \) shows a weak dependency on the density range used for the fit, with all the values between 1.70 \( \times 10^{11} \) cm\(^{-2} \) and 1.75 \( \times 10^{11} \) cm\(^{-2} \). The chosen value of \( n_p = 1.75 \times 10^{11} \) cm\(^{-2} \) is therefore a valid estimate since it is extracted considering a significant density range and further extending this range does not result in improvements in the error intervals.

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Further details of the oxidation process are considered a trade secret and are not reported in this paper.


The observed turn-on voltage of 1.22 V matches with the value of 1.15 V obtained by TCAD simulations considering the actual gate stack at cryogenic temperature and an intrinsic epitaxial layer. These results suggest there is no significant built-in charge-dependent threshold shift. Further agreement with experiments ($V_{TO} = 1.20$ V) is obtained taking into account a background doping density of $1 \times 10^{14}$ cm$^{-3}$.


