A scalable quantum computing architecture requires reproducibility and control over key qubit properties, such as resonance frequency, coherence time, etc. Variability in such parameters among qubits of a large-scale quantum computer would necessitate individual qubit characterization and control [1], while excessive variability could even make scaling impractical. In case of significant variability in the dephasing time, the qubit that decoheres the fastest might limit the overall performance.

Spin qubits hosted in Si quantum dots (QDs) [2] have been showing promise as a potential building block for a large-scale quantum computer [3], because of their compatibility with already existing complementary metal-oxide-semiconductor (CMOS) technology and the long coherence times available due to the presence of negligible nuclear spins in isotopically purified $^{28}$Si [4]. Single- [5–10] and two-qubit [11] gates have been demonstrated already. To move forward with increasing numbers of qubits [11,12–14], we have to study the possible sources that can cause variations in the coherence time and limit the performance of these qubits.

In this Rapid Communication, we provide a microscopic understanding of the dephasing time $T_2^*$ of Si QD spin qubits. We show that electrical noise modulates the electron $g$-factor through a spin-orbit interaction (SOI) and causes dephasing. Moreover, the atomic-scale details of the interface control the sensitivity of the $g$-factor to the electric field or noise and hence introduce variability in the $T_2^*$ times. We experimentally observe variations in the $g$-factors and their Stark shifts undergo variations due to these steps. We compare our theoretical predictions with experiments on QDs at a Si/SiO$_2$ interface, in which we observe significant differences in Stark shifts between QDs in two different samples. We also experimentally observe variations in the $g$-factors of one-electron and three-electron spin qubits realized in three neighboring QDs on the same sample, at a level consistent with our calculations. The dephasing times of these qubits also vary, most likely due to their varying sensitivity to charge noise, resulting from different interface conditions. More importantly, from our calculations we show that by employing the anisotropic nature of the spin-orbit interaction (SOI) in a Si QD, we can minimize and control these variations. Ultimately, we predict that the dephasing times of the Si QD spin qubits will be anisotropic and can be improved by at least an order of magnitude, by aligning the external dc magnetic field towards specific crystal directions, given other decoherence mechanisms do not dominate over charge noise.

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These SOI effects also make the qubits susceptible to electrical noise.

In a Si QD with a strong vertical electric field, the electrons are usually confined to only one interface. A monatomic shift in the location of this interface results in a sign inversion of the Dresselhaus coefficient, while the Rashba coefficient remains unchanged [19–21]. In practice, Si/SiGe or Si/SiO₂ interfaces certainly contain roughness, i.e., monatomic steps [23–25]. A nonideal interface with monatomic steps can be thought of as multiple smooth interface regions, where interfaces of neighboring regions are shifted by one atomic layer with respect to each other. Thus the neighboring regions will have opposite signs of β. An electron wave function spread over multiple such regions will witness multiple local β’s and the effective β will be a weighted average. Thus the presence of interface steps can change both the sign and magnitude of the effective Dresselhaus contribution to the electron g-factors in a Si QD [18]. In essence, local changes in the orientation of the chemical bonds of the atoms at the interface inside a dot may result in similar effects. To accurately understand these atomic-scale physics of the interface, here we use a spin-resolved $sp^3d^5s^*$ tight-binding model, where the effects of the SOI come out automatically based on the atomic arrangement of the QD, without any preassumption about the Rashba or Dresselhaus SOI.

Figure 1 shows how a monatomic step at the interface of a Si QD can affect the g-factors of the valley states and their electric field dependence, with an external magnetic field along the [110] crystal orientation, from atomistic tight-binding simulations. The distance between the dot center and the location of the edge of the interface step is denoted by $x_0$ [shown in Fig. 1(a)]. The dot radius is around 10 nm. So for $x_0 < -10$ nm the dot is completely on the left side of the step and has different g-factors ($g_- > g_+$) compared to that ($g_+ > g_-)$ for $x_0 > 10$ nm, when the dot is completely on the right side of the step, as seen in Fig. 1(b). For $-10$ nm $< x_0 < 10$ nm, the g-factors are a weighted average of those of the two sides based on the dot location. To understand this atomistic calculation we use an analytic effective mass model that relates $g_{\perp}$ in a Si QD, with the Rashba and Dresselhaus SOI [15,18]. We briefly summarize this model in the Supplemental Material [26]. For $B_{\text{ext}}$ along the [110] crystal orientation,

$$\delta g_{\perp}^{[110]} = g_{\perp}^{[110]} - g_{\perp} = \frac{2|e|\langle z\rangle}{\mu_B\hbar}(-\alpha_{\perp} + \beta_{\perp}). \quad (1)$$

Here, $g_{\perp} = 1.9937$ is the g-factor perpendicular to the valley axis [18,27], $|e|$ is the electron charge, $\langle z\rangle$ is the spread of the electron wave function along the vertical direction $z$ ([001]), and $\hbar$ is the reduced Planck constant. Now, in a Si QD, $\beta \gg \alpha$ [18,21], and so

$$\delta g_{\perp}^{[110]} \approx \frac{2|e|\langle z\rangle}{\mu_B\hbar} \beta_{\perp}. \quad (2)$$

As previously discussed, β has a different sign between the two sides of the step. When the location of the dot changes with respect to the step, the weighted average of the positive and negative β’s changes, which changes the g-factors.

**Figure 1.** Effect of interface steps on g-factors and their Stark shifts in a Si QD from an atomistic tight-binding calculation. (a) An electron wave function subject to an interface step. (b) Variation in the g-factors for both valley states ($g_-$ and $g_+$), as a function of $x_0$ for a vertical electric field $F_z = 28.5$ MV m⁻¹ [22]. When the electron is on the left (right) side of the step, $\beta_-$ is positive (negative) and $\beta_+$ is negative (positive), and we see $g_- > g_+$ ($g_- < g_+$). $F_z$ dependence of (c) $g_-$ and (d) $g_+$ for various $x_0$. The magnetic field used in the simulations of (b)–(d) is 1.4 T along the [110] crystal orientation and the monatomic step is parallel to the $y$ ([010]) direction.

Figures 1(c) and 1(d) show that the Stark shifts of the g-factors, as a function of the confining vertical electric field $F_z$, for both valley states are also affected by the presence of an interface step. The differential change in the g-factors with electric field, $dF_z$, can vary in both sign and magnitude depending on the location of the step. This behavior can also be explained by Eq. (2), with the change in β near an interface step. For example, in Fig. 1(c), for $x_0 \approx -10$ nm, the dot is completely on the left side of the step, where the $v_-$ valley state has positive $\beta$. Thus an increase in $\beta_-$ with increasing $F_z$ increases $g_-$ as well, hence a positive $\frac{dF_z}{dx_0}$. On the other hand, when the dot is completely on the right side of the step, at $x_0 \approx 10$ nm, $\beta_+$ is negative. Thus increasing $F_z$ increases $|\beta_+|$ but decreases $g_+$ and thus results in a negative $\frac{dF_z}{dx_0}$. For $-10$ nm $< x_0 < 10$ nm, $\frac{dF_z}{dx_0}$ changes gradually with $x_0$. We see a similar but opposite change for $g_+$ in Fig. 1(d).

Similar variations in the g-factors, and their gate voltage dependence, are measured in gate-defined quantum dots formed at a Si/SiO₂ interface for two different samples (A and B) with similar architecture. Figure 2(b) shows variations in one-electron and three-electron g-factors among $Q_1$, $Q_2$ and $Q_3$.
Q_3, in sample A [schematic shown in Fig. 2(a)]. We understand that the one-electron (three-electron) qubit corresponds to an electron occupying the lower (higher) energy valley state $v_-$ ($v_+$) [15]. We could not achieve three-electron spin resonance for $Q_2$ as it was strongly coupled to the other dots. In Fig. 2(c) we see that the $g_-$ of $Q_1$ has an opposite dependence on $F_z$ compared to that of the one QD in sample B. These observed variations in both the Stark shifts and the $g$-factors qualitatively agree with the theoretically predicted variations shown in Fig. 1. We therefore conclude that these experimentally observed variations are primarily due to different interface conditions associated with each of the QDs.

We also observe variations in the measured $T_2^*$ times, extracted by performing Ramsey experiments [26], for both valley states of the three QDs in sample A, as shown in Fig. 2(d).

The dephasing time due to nuclear spin fluctuations is given in Refs. [28,29], and in our samples, which employ an isotopically enriched $^{28}$Si substrate, these times are very long. In the absence of nuclear spin, we can relate $T_2^*$ times with $\langle \Delta F_i \rangle$ and the field fluctuation $\langle \Delta F_i \rangle$ due to nuclear spin fluctuations is calculated using computer-aided design (TCAD) simulations [26], we find $\Delta F_i = -5.34 \mu m^{-1}$ and $\Delta F_i = 0.2 \mu m^{-1}$, whereas $\Delta F_i = -3.52 \mu m^{-1}$ and $\Delta F_i = -1.52 \mu m^{-1}$ [26] for a 5-nm gate separation [Fig. 2(a)]. Here, $\Delta F_i^{\text{top}} (\Delta F_i^{\text{side}})$ is a voltage fluctuation in the top (side) gate. A larger gate separation will reduce $\Delta F_i^{\text{top}}$.

The observed variations in $T_2^*$ can be explained from the changes in $\delta x$ and $\delta z$ with interface step location, as shown in Figs. 3(a) and 3(b). When we compare the $T_2^*$ times between the two valley states of $Q_1$, we see $T_2^* (v_+; Q_1) \approx 1.7 T_2^* (v_-; Q_1)$, and from Ref. [15] we find $\delta x = 2.2 | \Delta F_i |$. This almost linear dependence of $\frac{\delta x}{\Delta F_i}$ shows the dominating contribution of $\Delta F_i$ on $T_2^*$ for $Q_1$. However, comparing Figs. 3(a) and 3(b) we see that $\frac{\delta x}{\Delta F_i}$ can be larger than $\frac{\delta z}{\Delta F_i}$ depending
Comparing Eqs. (2) and (5) we see that these variations and also negligible variations in along the [100] crystal orientation, all the qubits will have computer made of Si QDs. If the external magnetic field is times.

For steps parallel to the [110] and [100]. Though there are variations in g ± for [110] compared to that for [110]. Moreover, since β ± = α ± [18,21], δg ± itself will be much smaller for [100].

Figure 3(a) also compares variations in δg ± with x0 between Bext along [110] and [100]. Though there are variations in δg ± with x0 for Bext along [100], as shown by the inset of Fig. 3(a), these variations and also δg ± themselves are negligible, when compared to that along [110]. We see a similar reduction in δg ± (and its variability with x0) for Bext along [100] in Fig. 3(b). A variation of g ± with x0 will also be negligible for Bext along [100] [30], as shown in Fig. 3(c). Such phenomena will have a critical impact on the realization of a large-scale quantum computer made of Si QDs. If the external magnetic field is along the [100] crystal orientation, all the qubits will have negligible variations in g ±, δg ±, δg ±, and consequently in T 2∗ even in the presence of varying interface conditions. Very small |δF z | and |δF x | along [100] would also result in very long T 2∗ times.

In Fig. 3(d), the angular dependence of |δF z | = |δF x | + |δF y | for x0 = −6 nm, is shown. Here, T 2∗ = |δF z | |δF x | |μ B | Bext. As the monatomic step used in the calculation is parallel to the [010] crystal orientation, δg ± and thus T 2∗(ΔF z ) is negligible. A similar angular dependence of |δF y |

Now, a decrease in |δg ± | would also mean a reduced tunability of the g-factors, which is necessary for the selective addressing of individual qubits. However, an increase in T 2∗ times will result in a narrower electron spin resonance (ESR) linewidth, δF W H M = 2Δ1F z [9], which would then require a smaller difference in g-factors to individually address them.

Orienting the magnetic field along the [100] crystal orientation results in a Dresselhaus SOI with only off-diagonal components [26]. Therefore, electric field fluctuations, to first order, contribute to spin dephasing through the weaker Rashba SOI, ensuring a long T 2∗ time. At the same time, a resonant oscillating electric field can induce electric dipole spin resonance (EDSR) through the off-diagonal Dresselhaus coupling. Since T 2∗ is long under these conditions, coherent operations can be expected even for relatively weak EDSR driving strength, and without invoking the use of micromagnets [9].

To conclude, the presence of random monatomic steps at the interface of a Si QD can cause variations in both the sign and magnitude of the Dresselhaus SOI among neighboring Si QDs. As a result, the electron g-factors and their sensitivity to electric field should vary, which also leads to variability in the dephasing times among quantum dot spin qubits in Si. The extent of these variations is such that g-factors, Stark shifts, and dephasing times for the v± valley state can be larger than that of the v± valley state for some dots while vice versa for others, even with a similar range of vertical electric field across the dots. Likewise, the Stark shifts for the same valley state can change sign between dots. We also experimentally observe such variations, consistent with the theoretical understanding.

We further show that even in the presence of interface steps we can control and minimize these variations by taking advantage of the anisotropic nature of SOI in a Si QD. Importantly, we can increase T 2∗ times if we align the external magnetic field along the [100] crystal orientation, rather than along [110], which will also help to reduce the SOI-induced dephasing in Si QD devices with integrated micromagnets, as SOI also contributes to the g-factors in these devices [18]. These theoretical findings will guide future experiments to dig into the variability issues in detail and explore the role of the spin-orbit interaction in Si QDs.

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[30] Recently, we became aware of an experimental work [R. M. Jock et al., Nat. Commun. 4, 1768 (2013)] that measures the difference in g-factors between two neighboring QDs in a Si/SiO2 sample for different directions of Bext. Their findings validate our prediction. The authors also observe a further reduction in the g-factor difference for Bext along the [010] direction, due to the suppression of both the Rashba and Dresselhaus SOI along [010], while for [100] only the Dresselhaus SOI gets suppressed. However, we need at least some tunability of the g-factor in order to selectively address the qubits, which is possible through the weaker Rashba SOI along [100] but might not be possible along [010].