Epitaxial Profile Optimization for Valley Splitting Enhancement in Si/SiGe Spin-Qubits

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***Abstract*—The presence of two nearly degenerate conduction band valley states is a critical challenge for electron spin-qubits in silicon since it can lead to leakage of quantum information. Several heuristic strategies have been proposed to enhance the energy gap between these two states, also referred to as the *valley splitting*. In this work, we focus on the systematic optimization of the valley splitting in Si/SiGe heterostructures through the precise engineering of the Ge atom distribution within the quantum well, *i.e.*, epitaxial profile optimization. Our approach is based on envelope-function theory accounting for the effects of strain, compositional alloy disorder and non-trivial resonances. Our main result is a novel design, called the *modulated wiggle well*, that provides a reliably large deterministic enhancement of the valley splitting (assisted by shear strain). Previously proposed designs are recovered systematically as special cases of our constrained variational optimization problem.**

***Index Terms*—Silicon spin qubits, valley splitting, quantum dots, optimization.**

I. Introduction

Silicon-germanium (SiGe) heterostructures are a major candidate for realizing fully scalable quantum computers due to their long spin coherence times and compatibility with established semiconductor fabrication technology [1]. Experiments have demonstrated state initialization, readout as well as one and two-qubit gate operations exceeding the fault-tolerance threshold [2]. Scalable quantum computing architectures require coherent coupling of distant qubits to overcome crosstalk and quantum dot (QD) wiring limitations [3–5]. As a major step in this direction, coherent qubit transfer across the chip was recently demonstrated using conveyor-mode electron spin-qubit shuttles [6, 7].

A key challenge in strained Si/SiGe quantum wells (QWs) is the existence of two nearly degenerate conduction band valley states that can lead to leakage of quantum information outside of the computational Hilbert space. Several strategies have been proposed to enhance the energy splitting between the two valleys (*i.e.*, the *valley splitting*) such as sharp interfaces, Ge-spikes, oscillating Ge-concentrations ("wiggle well") and shear strain engineering [8, 9]. In all these approaches, one aims to tailor the Ge concentration profile $X\,(z)$ in the QW such that a resonance in the coupling of the two valley states is activated which eventually enhances the valley splitting. The inclusion of Ge, however, inevitably leads to alloy fluctuations that cause a statistical broadening of the valley splitting distribution in the device. Robust Si/SiGe qubits require a deterministic enhancement of the valley splitting that reliably exceeds the Zeeman splitting on the entire chip to avoid spin-valley hotspots [10]. This is especially important for shuttling-based quantum computing architectures [4], where the variability of the valley splitting is probed over large domains.

In this work, we consider the enhancement of the valley splitting as a constrained optimization problem on the epitaxial profile. Our approach is based on an envelope function theory that accounts for the effects of strain and alloy disorder [11].

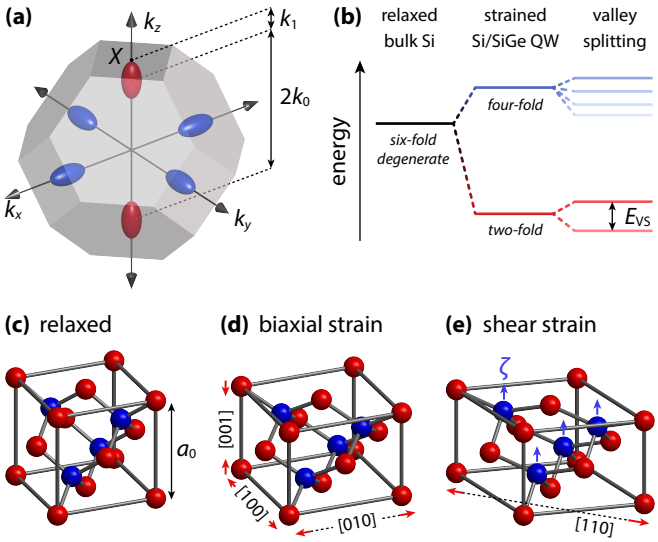

Fig. 1. **(a)** First Brillouin zone of the face-centered cubic (fcc) lattice. In Si/SiGe QWs, the degeneracy between the six equivalent conduction band minima in Si near the X-points is lifted by biaxial tensile strain. **(b)** Energy diagram for the conduction band ground states in Si/SiGe quantum dots. Biaxial strain due to lattice mismatch between Si and SiGe leads to a separation of the two valleys oriented along $[001]$ and $[00\bar{1}]$ from the other four conduction band ground state valleys. The heterostructure potential and alloy disorder finally lift the remaining degeneracies. **(c)-(e)** The effect of strain on the Si crystal structure. Shear strain along the [110] direction eliminates a nonsymmorphic crystal symmetry, which unlocks a low-frequency resonance mechanism that can be triggered by epitaxial profile design.

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II. Valley splitting model

The interaction of the two nearly degenerate low-energy valley states at the conduction band minimum $\mathbf{k} = \pm\mathbf{k}_0 \approx (0, 0, \pm 0.84) \times 2\pi/a_0$ of a biaxially (tensile) strained QW grown in [001] direction is described by the coupled envelope equation model [9, 12, 13]

$$\begin{pmatrix} H_0(\mathbf{r}) & V_c(\mathbf{r}) \\ V_c^*(\mathbf{r}) & H_0(\mathbf{r}) \end{pmatrix} \begin{pmatrix} \Psi_+(\mathbf{r}) \\ \Psi_-(\mathbf{r}) \end{pmatrix} = E \begin{pmatrix} \Psi_+(\mathbf{r}) \\ \Psi_-(\mathbf{r}) \end{pmatrix}, \quad (1)$$

where $\Psi_\pm(\mathbf{r})$ denotes the envelope wave functions of the corresponding valley states. Here, the valley splitting corresponds to the energy difference between the first excited state and the ground state. The Hamiltonian in (1) involves

$$H_0(\mathbf{r}) = -\frac{\hbar^2}{2m_t}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\hbar^2}{2m_l}\frac{\partial^2}{\partial z^2} + U(\mathbf{r}), \quad (2)$$

where m_l and m_t are the effective mass tensor components at the silicon conduction band minimum and $U(\mathbf{r})$ is the total confinement potential. The total confinement potential

$$U(\mathbf{r}) = U_{\mathrm{het}}(\mathbf{r}) + U_{\mathrm{QD}}(x, y) + U_F(z), \quad (3)$$

describes the effects of both the epitaxial heterostructure and the electrostatic fields induced by the metal gates at the top surface of the device. The heterostructure potential $U_{\mathrm{het}}(\mathbf{r})$ describes the potential induced by the Ge atoms in the SiGe alloy, *i.e.*, a type-II Si/SiGe QW with random alloy disorder. The average heterostructure potential is proportional to the nominal Ge concentration profile, $\langle U_{\mathrm{het}}(z)\rangle \propto X(z)$. We assume a harmonic QD confinement potential induced by the gate electrodes

$$U_{\mathrm{QD}}(x, y) = \frac{m_t}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2\right), \quad (4)$$

where ω_x and ω_y describe the lateral extension of the QD and thus the orbital splitting $\Delta E_{\mathrm{orb}} = \min(\hbar\omega_x, \hbar\omega_y)$. In the limiting case of $\omega_x = \omega_y$, the QD takes a circular shape. Finally, we assume a constant electric field F along the growth direction, which induces the potential

$$U_F(z) = -e_0 F z, \quad (5)$$

where e_0 is the elementary charge. The intervalley coupling $V_c(\mathbf{r})$ in (1) is described by

$$V_c(\mathbf{r}) = \mathrm{e}^{-2i\mathbf{k}_0\cdot\mathbf{r}} u^*_{+\mathbf{k}_0}(\mathbf{r})\, u_{-\mathbf{k}_0}(\mathbf{r})\, U(\mathbf{r}), \quad (6)$$

which involves the lattice-periodic part of the Bloch factors at the two valleys, $u_{\pm\mathbf{k}_0}(\mathbf{r})$. In first-order degenerate perturbation theory, the valley splitting $E_{\mathrm{VS}} = 2|\Delta|$ is determined by the complex-valued inter-valley coupling parameter [11]

$$\Delta = \int \mathrm{d}^3 r\, V_c(\mathbf{r}) \left|\Psi_0(\mathbf{r})\right|^2, \quad (7)$$

where $\Psi_0(\mathbf{r})$ is the envelope function of the twofold degenerate ground state of the single valley Hamiltonian $H_0(\mathbf{r})$.

TABLE I
Parameter values used in the computations

Symbol	Description	Value
ΔE_c	Si/Ge conduction band offset	$0.5\,\mathrm{eV}$
X_b	Mean barrier Ge concentration	0.3
$\hbar\omega_x, \hbar\omega_y$	Orbital splitting energy (circular QD)	$3.0\,\mathrm{meV}$
F	Electric field strength	$5\,\mathrm{mV/nm}$
h_{QW}	Quantum well thickness[a]	$75\,\mathrm{ML}$

[a] Given in monolayers ($\mathrm{ML} = a_0/4$) of relaxed Si.

III. Strain and Resonances

The model described above predicts that a large valley splitting can be achieved when the confinement potential $U(\mathbf{r})$ contains components oscillating at a spatial frequency of $2k_0$, owing to the presence of the exponential term in the expression for $V_c(\mathbf{r})$, see (6). This principle underpins the design of so-called *wiggle well* heterostructures, in which the Ge concentration profile $X(z)$ is engineered to oscillate at this resonant frequency,

$$\langle U_{\mathrm{het}}(z)\rangle \propto X(z) \propto \cos(qz), \qquad q = 2k_0. \quad (8)$$

Such devices are challenging to fabricate since $2k_0 \approx 1.7 \times 2\pi/a_0$ corresponds to rapid oscillations at the length scale of about 2.4 monolayers.

In the presence of shear strain, a second, lower-frequency resonance becomes accessible at $2k_1 \approx 0.32 \times 2\pi/a_0$. This arises due to the folding of the $2k_0$ component in the spectral content of $V_c(\mathbf{r})$, back into the first Brillouin zone, such that $2k_1 = 4\pi/a_0 - 2k_0$. In unstrained silicon, this resonance is suppressed due to symmetries of the crystal and the Bloch factors $u_{\pm\mathbf{k}_0}(\mathbf{r})$ [13].

Shear strain modifies the lattice and the associated Bloch factors, thereby activating the $2k_1$ resonance. In our work, we compute the band structure coefficients—including Bloch factors, effective masses, and conduction band minima—using a non-local empirical pseudopotential model (EPM) [14]. A key advantage of the EPM is its natural capability to describe the effects of homogeneous strain, modeled as a displacement of ionic positions

$$\mathbf{R}_i' = (I + \varepsilon)\,\mathbf{R}_i, \quad (9)$$

where ε is the strain tensor. Incorporating strain into EPM calculations involves several steps: adjusting reciprocal lattice vectors to $\mathbf{G}_i' \approx (I - \varepsilon)\,\mathbf{G}_i$, modifying the primitive cell volume to $\Omega_p' \approx (1 + \mathrm{tr}(\varepsilon))\,\Omega_p$, interpolating atomic pseudopotentials at the strained lattice points, and including internal ionic displacements that describe sublattice shifts [15]. These effects are illustrated schematically in Fig. 1. In this work, a weak homogeneous shear strain of $0.1\,\%$ is assumed in the QW layer.

IV. Disorder and Statistics

Compositional alloy disorder in the heterostructure is described using a statistical model for the distribution of Si and

Ge atoms in the device depending on the local concentration $X(\mathbf{R}_i)$ at each lattice site $\mathbf{R}_i$. The model potential reads [11]

$$U_{\text{het}}(\mathbf{r}) = \Delta E_c \, \Omega_a \sum_i N_i \, \delta(\mathbf{r} - \mathbf{R}_i), \tag{10}$$

where ΔE_c is the Si/Ge conduction band offset, Ω_a is the atomic volume and $N_i \sim \text{Binomial}(p = X(\mathbf{R}_i))$ is a random variable determining the atomic species depending on the nominal epitaxial profile X. The confinement potential can therefore be decomposed into a sum of the average potential and the fluctuations from the average,

$$U(\mathbf{r}) = \langle U(\mathbf{r}) \rangle + \delta U(\mathbf{r}). \tag{11}$$

The above potential also renders the inter-valley coupling parameter (7) a stochastic quantity, with a deterministic component Δ_{det} and a random component Δ_{rand},

$$\Delta = \Delta_{\text{det}} + \Delta_{\text{rand}}, \tag{12}$$

where

$$\Delta_{\text{det}} = \int \mathrm{d}^3 r \, \mathrm{e}^{-2i\mathbf{k}_0 \cdot \mathbf{r}} u^*_{\mathbf{k}_0}(\mathbf{r}) \, u_{-\mathbf{k}_0}(\mathbf{r}) \, \langle U(\mathbf{r}) \rangle \, |\Psi_0(\mathbf{r})|^2,$$

$$\Delta_{\text{rand}} = \int \mathrm{d}^3 r \, \mathrm{e}^{-2i\mathbf{k}_0 \cdot \mathbf{r}} u^*_{\mathbf{k}_0}(\mathbf{r}) \, u_{-\mathbf{k}_0}(\mathbf{r}) \, \delta U(\mathbf{r}) \, |\Psi_0(\mathbf{r})|^2.$$

Using the central limit theorem, Δ obeys a circular symmetric normal distribution in the complex plane with (approximately) independent and identically distributed real and imaginary parts

$$\text{Re}(\Delta) \sim \text{Normal}\left(\mu = |\Delta_{\text{det}}| \cos(\Theta), \sigma^2 = \frac{1}{2}\Gamma\right), \tag{13}$$

$$\text{Im}(\Delta) \sim \text{Normal}\left(\mu = |\Delta_{\text{det}}| \sin(\Theta), \sigma^2 = \frac{1}{2}\Gamma\right), \tag{14}$$

with mean $\Delta_{\text{det}} = |\Delta_{\text{det}}| \exp(i\Theta)$ and covariance

$$\Gamma = \langle |\Delta_{\text{rand}}|^2 \rangle \tag{15}$$

The mean μ and variance σ^2 of the normal distributions in (13)–(14) are determined by $\Delta_{\text{det}} = \Delta_{\text{det}}(X, \Psi_0)$ and $\Gamma = \Gamma(X, \Psi_0)$, which are both complex functionals of the Ge concentration profile $X(z)$, the electron density distribution $|\Psi_0(\mathbf{r})|^2$ and (strain-dependent) band structure parameters [11]. A large mean is due to a deterministic enhancement of the valley splitting, whereas a large variance is caused by a strong random component.

V. Optimization

We seek for an epitaxial profile in the QW that guarantees a *reliably* large valley splitting by providing an optimal balance between a large deterministic and a small disorder-induced contribution. We formulate this objective as a constrained optimization problem for the Ge concentration profile $X(z)$

$$\max_X \frac{|\Delta_{\text{det}}(X, \Psi_0)|^2}{\Gamma(X, \Psi_0)} \tag{16a}$$

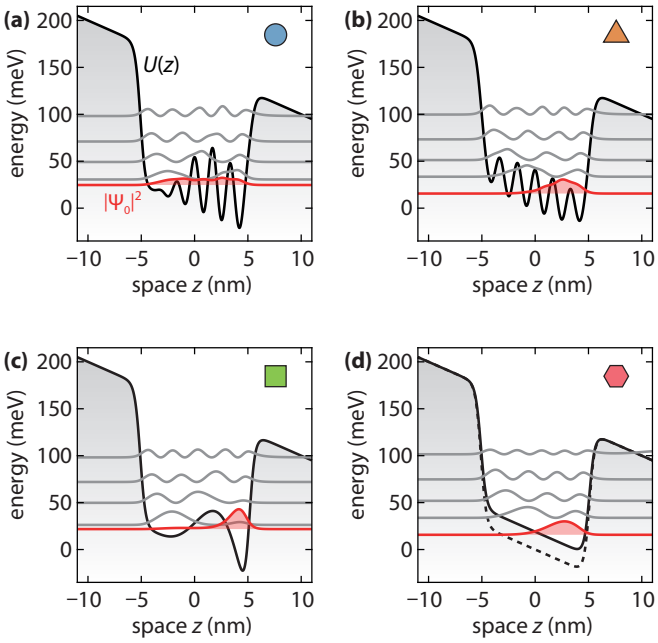

Fig. 2. Epitaxial profiles obtained from variational optimization of the valley splitting for different cost functionals. All epitaxial profiles are constrained to a Ge budget of $X_{\text{mean}} = 5\,\%$ within the QW. **(a)** Modulated wiggle well computed by maximizing Eq. (16a) with $k_c = 0.38 \times 2\pi/a_0$. **(b)** Conventional wiggle well for comparison. Within the QW, the Ge profile is $X(z) \propto \cos(2k_1 z)$. **(c)** Ge spike-like structure obtained by maximizing $|\Delta_{\text{det}}|$ under an intermediate frequency cutoff $k_c = 0.06 \times 2\pi/a_0$. **(d)** Flat Ge concentration, computed by maximizing Eq. (16a) under a stringent frequency cutoff $k_c = 0.01 \times 2\pi/a_0$.

subject to the constraints

$$H_0(X)\,\Psi_0(\mathbf{r}) = E_0 \Psi_0(\mathbf{r}), \tag{16b}$$

$$0 \le X(z) \le X_b, \tag{16c}$$

$$\frac{1}{h_{\text{QW}}} \int_{\text{QW}} \mathrm{d}z \, X(z) = X_{\text{mean}}, \tag{16d}$$

$$\tilde{X}(|k| > k_c) = 0. \tag{16e}$$

The constraints enforce the envelope wave function to be the ground state of the single-valley Schrödinger equation (16b), a restriction of the local Ge concentration within the admissible range (16c) and a fixed mean Ge content in the QW (16d), where h_{QW} denotes the thickness of the QW. The last condition (16e) is a spectral constraint that excludes high frequency components above the cutoff wave number k_c.

To compute the optimized epitaxial profiles, the constrained optimization problem is first converted into an unconstrained optimization problem using the Lagrange multiplier method. The constraints on the Ge concentration profile (16c)–(16d) are included as penalty terms in the target functional of (16a). The gradient of the target functional is computed by solving the adjoint equation, taking the spectral filter according to (16e) into account. The epitaxial profile $X(z)$ is iteratively updated using the L-BFGS algorithm [16], until convergence is reached.

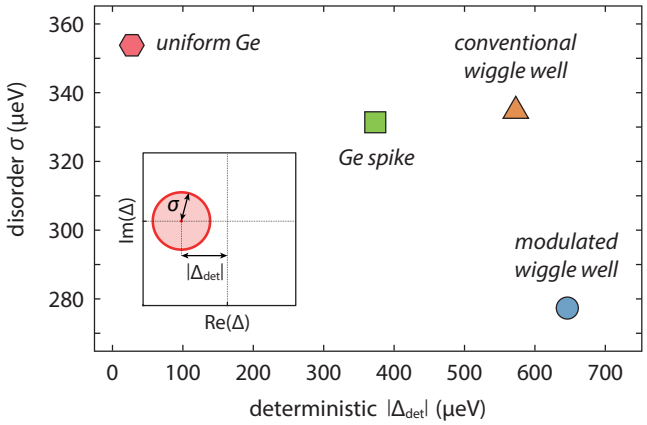

Fig. 3. Computed values of the deterministic contribution $|\Delta_{\mathrm{det}}|$ and the disorder induced contribution contribution $\sigma^2 = \Gamma/2$ to the intervalley coupling parameter for the structures in Fig. 2. The inset shows a sketch of the circular normal distribution of Δ in the complex plane.

VI. Results

The results of the variational optimization procedure for different constraint parameter sets and various optimization goals, *i.e.*, adaptations of Eq. (16a), are shown in Fig. 2. The variational approach recovered a number of previously known profiles but also new, enhanced designs. The associated deterministic and disorder induced contributions to the valley splitting are plotted in Fig. 3.

Our main result is the *modulated wiggle well* assisted by shear strain shown in Fig. 2 (a). The optimization scheme converges to a Ge concentration profile that has a dominant spectral component at $2k_1$, similar to the conventional (long-period) wiggle well, see (8). In contrast to the conventional wiggle well, however, the modulated wiggle well is adapted to the local electric field and yields both an enhanced deterministic and a reduced random contribution to the valley splitting, as can be seen in Fig. 3. Furthermore, the optimized structure shows a strong electric field dependency enabling enhanced control and tunability of the valley splitting. The design is compatible with state-of-the-art fabrication technology [17].

In addition, in Fig. 2 (c), we plot the computed profile for an intermediate frequency cutoff k_c, which prevents the optimized Ge concentration from oscillating as rapidly as the structures of Figs. 2(a)–(b). This profile resembles the previously proposed Ge spike structure [8]. Finally, when imposing a stringent frequency cutoff, we obtain a QW with uniform Ge concentration shown in Fig. 2 (d). The comparison in Fig. 3 reveals that this structure has the smallest deterministic component and the main contribution to the valley splitting arises from the disorder induced component.

VII. Summary

We have developed a variational optimization framework to compute optimal Ge concentration profiles in strained SiGe quantum wells for maximizing the valley splitting. Our approach recovers previous heuristic strategies and enables systematic exploration of the design space under physical constraints. Our method reproduces known structures such as the wiggle well and Ge spike and produces improved designs, notably the modulated wiggle well, which offers enhanced deterministic splitting, reduced variability, and strong tunability. These results are compatible with current epitaxial growth capabilities and provide a useful design tool for engineering valley splitting in silicon-based quantum devices.

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