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Electroelastic Hyperfine Tuning of Phosphorus Donors in Silicon

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We demonstrate an electroelastic control of the hyperfine interaction between nuclear and electronic spins opening an alternative way to address and couple spin-based qubits. The hyperfine interaction is measured by electrically detected magnetic resonance in phosphorus-doped silicon epitaxial layers employing a hybrid structure consisting of a silicon-germanium virtual substrate and a piezoelectric actuator. By applying a voltage to the actuator, the hyperfine interaction is changed by up to 0.9 MHz, which would be enough to shift the phosphorus donor electron spin out of resonance by more than one linewidth in isotopically purified ^{28}Si.

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Triggered by the proposal of Kane for a solid-state based quantum computer [1], the spins of donors in silicon have drawn attention as qubits [2,3] because of their long coherence times [4,5], their compatibility with silicon technology, and their scalability. Significant technological progress towards the spatial positioning of single donors has been made [6,7], and the single-shot readout of an electron spin has been demonstrated [8]. One key issue towards realizing Kane's proposal is addressing individual spins within a qubit array. It has been proposed to apply static and microwave magnetic fields globally and to shift single spins in and out of resonance by Stark tuning the hyperfine (hf) interaction of electrons and nuclei via locally applied electric fields (A gates). Bradbury *et al.* demonstrated the Stark tuning for ^{121}Sb in ^{28}Si, achieving a maximum resonance-field shift of $\approx 0.9\ \mu$T, corresponding to 25 kHz [9] limited by field ionization.

In this Letter, we propose an alternative approach, where the A gates are realized electroelastically by piezoelectric nanoactuators. This design has the potential for significantly larger shifts of the hf interaction, circumvents the risk of donor ionization, and adds another (mechanical) degree of freedom to the quantum computer architecture. A possible realization of an elemental two-qubit processor with electroelastic A gates, including the strain field induced by one of the actuators, is shown in Fig. 1. To estimate the strain distribution, we assumed elastically isotropic silicon with a Poisson ratio of 0.28 and modeled the actuator by a homogeneously loaded circle with a diameter equal to the width of the actuator, in analogy to Ref. [10]. The isolines shown in Fig. 1 indicate the magnitude of the out-of-plane strain ε_{33} normalized to its maximum value, demonstrating that the strain could be generated sufficiently locally by nanoactuators. The strong effect of strain on the exchange interaction of spatially separated donors [11] suggests that the exchange (J) coupling of the qubit pair is also influenced by the electroelastic A gates shown in Fig. 1. This could be exploited for J tuning in a hybrid gate system, illustrated in Fig. 1, or possibly even for all-elastical J tuning. Here we demonstrate, in a proof-of-concept experiment, an electroelastically induced shift of the ^{31}P hf interaction by 0.9 MHz, corresponding to 30 μT. Because the hf interaction is most susceptible to strain if the crystal is already prestrained to some extent [12], we demonstrate the electroelastic hf tuning in a Si film on a SiGe virtual substrate cemented to a piezoelectric actuator.

The spin Hamiltonian of a ^{31}P donor in silicon in the presence of an external magnetic field is given by $\hat{H} = g\mu_B B_0 \hat{S}_z + a\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{I}}$, with the electronic g factor of the donor, the Bohr magneton μ_B, the external magnetic flux density B_0 defining the quantization direction z, the electron and nuclear spin operators $\hat{\boldsymbol{S}}$ and $\hat{\boldsymbol{I}}$, and the z component of the electron spin operator $\hat{S}_z$; $a \sim |\psi(0)|^2$ is the Fermi contact hf interaction between the electron and nuclear spin, and $\psi(0)$ is the donor wave function at the

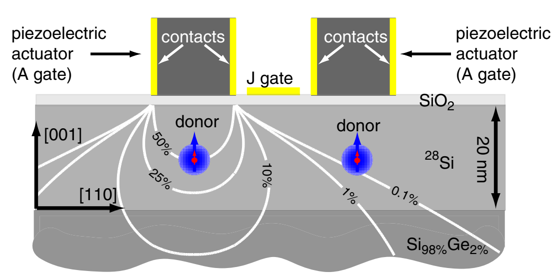

FIG. 1 (color online). Illustration of a modified architecture for a spin-based Si quantum computer with electroelastic A gates, realized by piezoelectric nanoactuators. These actuators strain the crystal in the vicinity of the donor, which alters the hf coupling between nuclear spin (small red arrow) and electronic spin (large blue arrow) and thus allows us to shift the donor spins in and out of resonance. The isolines show the distribution of the out-of-plane strain ε_{33}, normalized to its maximum value, as described in the text. The ^{28}Si layer is grown on a virtual SiGe substrate to enhance the efficiency of the electroelastic gates.

nucleus [13]. Because of the nuclear spin $I = 1/2$ of ^{31}P, the hf coupling gives rise to two resonance lines split by $A_{\text{hf}} = a/g\mu_B = 4.2$ mT in the limit of high magnetic fields, with $g = 1.9985$ in the absence of strain [14].

The influence of strain on the hf interaction was initially described by the valley repopulation model (VRM) [13]. For shallow donors in Si, the wave function for donor-bound electrons is of the form $\psi = \sum_{\mu=1}^{6} \alpha_\mu \phi_\mu$, where ϕ_μ is the product of the conduction-band Bloch function and the hydrogen-like envelope function at the μth conduction-band valley; $|\alpha_\mu|^2$ is the probability of finding the electron in the μth valley. If the crystal is strained, the energy levels of the valleys change, which results in their repopulation. This alters the wave function at the nucleus and therefore the hf constant [13]. For uniaxial strain along the [001] direction, the VRM predicts a change of the hf constant according to $A_{\text{hf}}(\chi) = A_{\text{hf}}(0)\frac{1}{2}[1 + (2 + \frac{1}{3}\chi) \times (\chi^2 + \frac{4}{3}\chi + 4)^{-(1/2)}]$ [13], as shown in Fig. 2 as a function of the out-of-plane component of the strain tensor ε_{33}. Here, $\chi = \Theta_u \varepsilon_{33}(1 + C_{11}/2C_{12})/3\Delta_C$ is the so-called valley strain [13], $C_{11} = 165.5$ GPa and $C_{12} = 63.9$ GPa are the elastic constants of Si [15], and $6\Delta_C = 12.96$ meV is the energy gap between the ^{31}P ground state and the doublet excited state in the unstrained material [16]. As Fig. 2 suggests, the hf interaction can be engineered by, e.g., pseudomorphically growing thin Si layers on top of SiGe virtual substrates [12]. For (001)-oriented substrates, this results in a biaxial tensile in-plane strain $\varepsilon_{11} = \varepsilon_{22} = (a_{\text{Si}} - a_{\text{SiGe}})/a_{\text{Si}}$, where a_{Si} and a_{SiGe} are the lattice constants of Si and the relaxed SiGe lattice, respectively. The indices of the strain components refer to the cubic axes of Si. The out-of-plane component of the strain tensor is $\varepsilon_{33} = -2\varepsilon_{11}C_{12}/C_{11}$ [12].

To achieve *in situ* tunable strain, we use the hybrid structure shown in Fig. 3, where the SiGe heterostructure

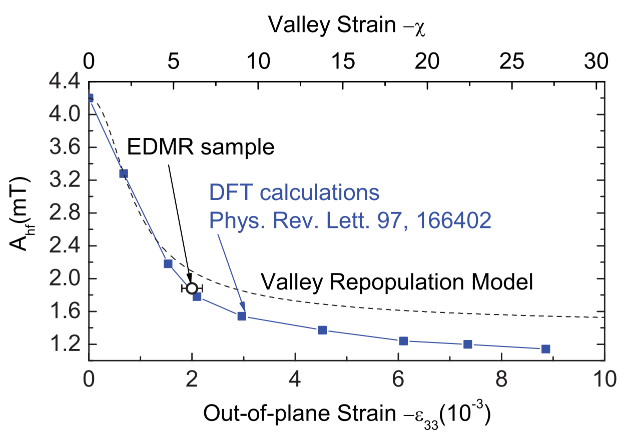

FIG. 2 (color online). Hyperfine splitting as a function of the out-of-plane strain according to VRM (dashed line) and DFT (solid squares) calculations; the solid line is a guide to the eye. The hf interaction of the sample studied with EDMR (open circle) is reproduced by the DFT calculations.

is cemented to a piezoelectric actuator such that the dominant elongation axis of the actuator is along the crystallographic [110] direction of Si. The actuator thus induces the strains ε_L and ε_T along [110] and [1$\bar{1}$0], respectively, resulting in a change of the in-plane strain components $\Delta\varepsilon_{11} = \Delta\varepsilon_{22} = (\varepsilon_L + \varepsilon_T)/2$ and $\Delta\varepsilon_{12} = (\varepsilon_L - \varepsilon_T)/2$ [17]. For the out-of-plane component we find $\Delta\varepsilon_{33} = -2\Delta\varepsilon_{11}C_{12}/C_{11}$, calculated from Hooke's law. While the VRM is accurate for moderate strain [13], Huebl *et al.* demonstrated that in order to account for the hf interaction for $-\varepsilon_{33} \gtrsim 1.5 \times 10^{-3}$, density functional theory (DFT) calculations are necessary (squares in Fig. 2) [12].

To experimentally demonstrate the electroelastic hf tuning, we start from a 15 nm-thick P-doped Si layer with $[\text{P}] \approx 1 \times 10^{17}$ cm^{-3} pseudomorphically grown by chemical vapor deposition on a relaxed virtual SiGe substrate [12], consisting of a 30 Ω cm Si:B (001) wafer, a 0.3 μm-thick Si buffer, and SiGe epilayers with stepwise increased Ge concentration, the final layer being 2 μm thick with a Ge content of 7 at. %. According to Vegard's law, this results in an out-of-plane strain of $\varepsilon_{33} = -2 \times 10^{-3}$ [18], corresponding to the open circle in Fig. 2. For photoconductivity measurements, an interdigit Au-Cr contact structure (cf. Fig. 3) was processed on the Si:P layer with optical lithography. After a 2 μm-thick insulating layer, consisting of hard-baked SU8 2002 photoresist, a coplanar stripline (CPS) was patterned on the device, as shown in Fig. 3. The CPS is terminated with a single loop, which allows for broadband generation of microwave Oersted fields. The Si substrate was then polished to a thickness of ≈ 80 μm, and a 600 nm-thick Si_3N_4 layer was deposited on the backside in order to prevent an electrical shortcut of the piezoelectric actuator when illuminating the Si heterostructure. The Si substrate was cemented on a "PSt 150/2 × 3/20" piezoelectric actuator (Piezomechanik München) with the two-component epoxy MBond 600 (Vishay Inc.) and annealed for 4 h at 120 °C in air. Measurements with strain gauges, performed at the same type of actuator at $T = 5$ K, revealed a linear voltage dependence of the actuator-induced strain [17].

The hybrid was mounted to a sample holder made out of a Rogers 3000 printed circuit board, which provides four dc contacts for the piezoelectric actuator and the interdigit structure, as well as a CPS with 50 Ω line impedance

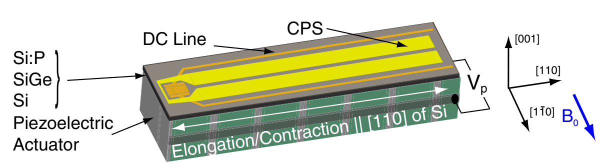

FIG. 3 (color online). The hybrid device used for the EDMR measurements allows for on-chip microwave magnetic field generation by a loop-terminated CPS, photoconductivity measurements, and application of voltage-controlled strain. Strain along the [110] direction results in in- and out-of-plane strain components.

merging into a coplanar waveguide [19]. To measure the hf interaction, we performed electrically detected magnetic resonance (EDMR) measurements [20], monitoring resonant changes of the photoconductivity caused by a spin-dependent recombination process between the ^{31}P donor electrons and P_{b0} interface states at the Si/SiO_2 interface [21]. The experiments were performed in a He-gas flow cryostat at 2.2 K under illumination with white light from a tungsten lamp. The magnetic field was oriented along $[1\bar{1}0]$, as indicated in Fig. 3. To isolate the hf-split ^{31}P resonances from other signals and to be insensitive to strain-induced g-factor shifts, the measurements were carried out at a microwave frequency of $\nu = 970$ MHz. The microwave power applied to the sample holder was 100 mW. Resonant changes of the photocurrent ΔI were detected using a current amplifier and lock-in detection, modulating the magnetic field with an amplitude of 0.2 mT at 25 kHz. The dc bias electric field applied to the interdigit structure was 0.5 kV/cm, resulting in a photocurrent of 12 μA. We applied a voltage of ± 200 V to the actuator; to cancel the influence of slow drifts, the polarity of the voltage was reversed before each sweep by ramping the voltage with a ramp time of 10 s, allowing for the system to equilibrate. To improve the signal-to-noise ratio, we averaged over 150 pairs of field sweeps; the total measurement time was 10 h. Each field sweep was normalized to the absolute photocurrent I during that sweep.

The spectra accumulated in two data sets for $V_p = +200$ V and $V_p = -200$ V are shown in Fig. 4(b). As discussed in Ref. [12], the central line is a superposition of two P_{b0} resonances with $g = 2.0042$ and $g = 2.0081$ [22] for this field orientation and a resonance presumably due to conduction-band electrons at $g = 1.9994$ [23], which are not spectrally resolved at $\nu = 970$ MHz. The two ^{31}P hf lines are isolated from the central line and are split by 1.88 mT, which is somewhat less than in Ref. [12] probably due to an additional strain, induced by the different thermal expansion coefficients of Si and the actuator. Because of the magnetic field modulation, the spectra take the form of a first derivative of a resonance curve. In Fig. 4(a), the low-field ^{31}P resonance is magnified, and a strain-induced shift of the resonance field by 17 μT can be seen clearly, which is more than 1 order of magnitude larger than the 0.9 μT achieved by Stark tuning [9]. The inset of Fig. 4 demonstrates the linearity of the low-field ^{31}P resonance-field shift ΔB_{low} with the actuator voltage. The hf change can be observed more distinctly in Fig. 4(c), where the dots represent the difference of the measured data shown in (b). The lines occurring at the ^{31}P resonance fields resemble the second derivative of a resonance curve, differing in sign. This is due to the fact that an increase (decrease) of the hf coupling shifts the resonance field of the low-field resonance to a smaller (larger) value and vice versa for the high-field resonance. Note that a temperature-induced hf change [24] can be ruled out because it would

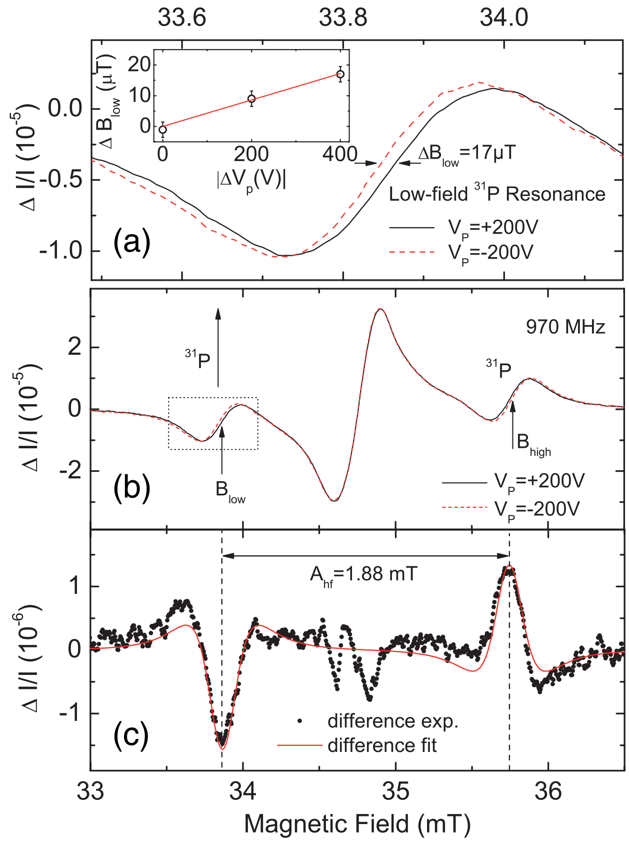

FIG. 4 (color online). The EDMR spectra obtained at actuator voltages $V_p = \pm 200$ V are shown in (b). In (a) the low-field ^{31}P resonance is magnified, demonstrating the actuator tuning of the hf interaction, which is a linear function of $|\Delta V_p|$, as shown in the inset. The spectra in (b) have been fitted by Lorentzian lines, and the difference of the fits is shown in (c) together with the difference of the measured data.

not reverse its sign upon changing the voltage polarity. To obtain the quantitative difference in the hf interaction for the obtained data sets, we performed a free fit to the spectrum with $V_p = 200$ V, using Lorentzian lines for the ^{31}P resonances and two Lorentzian lines (one broader and one narrower) for the central line [12]. With the same set of parameters the spectrum obtained at $V_p = -200$ V was fit, only varying the resonance field positions B_{low} and B_{high} (cf. Fig. 4) of the ^{31}P lines. The difference of the fits is represented by the solid line in Fig. 4(c). We find that the hf interaction A_{hf} is changed by (30 ± 5) μT for $|\Delta V_p| =$ 400 V. This change, as well as the absolute value $A_{\text{hf}} = 1.88$ mT, obtained from $A_{\text{hf}} = [A_{\text{hf}}(200\text{ V}) + A_{\text{hf}}(-200\text{ V})]/2$, is in agreement with the DFT calculations, assuming a voltage dependence of the actuator-induced strain of $\Delta\varepsilon_L = 3.3 \times 10^{-7}$/V and $\Delta\varepsilon_T = -7 \times 10^{-8}$/V, which are typical values for this type of actuator [17]. The different intensities of the two ^{31}P lines in Fig. 4(c) can be quantitatively accounted for by considering the Breit-Rabi diagram for low magnetic fields where the hf interaction causes some level mixing [25]. Note that according to theoretical calculations, a strain-induced g-factor shift of ^{31}P leads to a resonance-field shift of below 0.1 μT at $\nu = 970$ MHz [13]. The asymmetry of the ^{31}P second-derivative lines in Fig. 4(c) is due to a slight asymmetry in the measured line shapes, which was not taken into account by the fit.

In conclusion, we have demonstrated a voltage-controlled shift of the ^{31}P hf interaction by (30 ± 5) μT in a Si thin film on a SiGe/piezoelectric actuator hybrid, achieving a resonance-field shift of 17 μT, exceeding the linewidth of ^{31}P in ^{28}Si (8 μT) [5]. For quantum computation, the selectivity with which single spins can be addressed is most relevant. It is expected to be limited by microwave power broadening rather than by the linewidth of a single spin, thus requiring long low-power pulses; a 1100 μs-long π pulse, e.g., would flip a spin which is shifted off resonance by 17 μT with a probability of less than 10^{-6}, as required for resilient quantum computation [26]. Virtual substrates with optimized epitaxial strain would further increase the strain-induced resonance shift by roughly a factor of 3 according to the DFT calculations; this could be achieved by reducing the Ge content to 2 at. %. The effect could be further increased by 2 orders of magnitude for ^{209}Bi ($I = 9/2$) donors in Si, when exploiting the stronger hf coupling (52.7 mT) [14] and the spin projections of $\pm 9/2$. Since decoherence of ^{209}Bi electron spins appears to be as slow as that of ^{31}P [27], the corresponding reduction of the π pulse time in ^{28}Si^{209}Bi to 10 μs should allow us to perform up to 10^5 single-gate operations within 1 sec. Considering the progress in the nanofabrication of ferroelectrics [28], actuators with lateral dimensions of below 10 nm are realistic. The response time of such nanoactuators is expected to be comparable to that of electric gates, since it is limited by the contact capacitances rather than by the velocity of sound in solids, making electroelastic gates a promising approach within the framework of Kane's proposal for a quantum computer.

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