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Interqubit coupling based on indirect interaction of ^{31}P nuclear spins with electrons localized in a ^{28}Si nanowire

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Abstract

We suggest a new method of quantum information processing based on the precise placing of ^{31}P atoms in a quasi-one-dimensional ^{28}Si nanowire using isotope engineering and neutron-transmutation doping of the grown structures. In our structure, interqubit entanglement is based on the indirect interaction of ^{31}P nuclear spins with electrons localized in a nanowire. This allows one to control the coupling between distant qubits and between qubits separated by non-qubit neighboring nodes. The suggested method enables one to fabricate structures using present-day nanolithography. Numerical estimates show the feasibility of the proposed device and method of operation.

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1 Introduction

There is great scientific and commercial interest in the development of quantum computation (QC) and the creation of computational devices based on the principles of quantum logic. Several different schemes for QC have been proposed to date (see, for example, [1] and references therein). One of the exciting avenues, potentially compatible with the vast fabrication capabilities of modern semiconductor technology, relies on the encoding of information in the electron or nuclear spins present in semiconductor nanostructures, leading to a spin-based semiconductor quantum computer [2–6].

The most developed model of the nuclear spin quantum computer is the Kane suggestion [4] to use a precisely located array of phosphorous donors introduced into Si. In this proposal, the nuclear spin $^1/_2$ of ^{31}P is used as a qubit, while a donor electron together with an overlying gate (A-gate) separated from the donor by a SiO_2 or $Si_{0.85}Ge_{0.15}$ barrier, provides single-qubit operation using an external magnetic field and pulses of radio-frequency radiation. The interqubit coupling is determined by the overlap of the electron wave functions and is controlled by metallic gates (J-gates) midway between the A-gates. The overlap of wave functions of localized electrons in Si drops very rapidly with distance r, $\exp(-2r/a_B)$, where a_B is the radius of localization (for P in Si, $a_B \approx 2.5$ nm), therefore the interqubit distance r between P atoms must be small (less than 20 nm) to allow overlap.

Experimental realization of the suggested model presents a number of difficulties. We focus here on two problems: (1) placing single P donors into the Si substrate at a precise depth underneath the barrier and (2) the necessity to increase significantly the interqubit distance r to have room enough to arrange the metallic gates. This means that mechanisms other than the direct overlap of the electron wave functions have to be chosen for the coupling of adjacent nuclear spin qubits.

To solve these problems, we suggest the novel technology based on epitaxial growth of Si and SiGe layers from isotopically engineered Si and Ge sources followed by neutron-transmutation doping of the grown structures. We also describe the mechanism of indirect interqubit coupling based on the arrangement of qubits in a mesoscopic quasi-one-dimensional wire. This mechanism allows one to control the coupling between qubits separated by large distances r (200 nm or even more), which permits the fabrication of metallic gates by means of the modern lithography. Moreover, the suggested mechanism of indirect coupling allows entanglement passing over non-qubit nodes in an array of qubits. We also present the numerical estimates which justify the feasibility of the proposed device and method of operation.

2 Precise placement of P atoms into Si

Two methods, "bottom-up" and "top-down", had prevoiusly been suggested for the precise placing of P atoms into Si (for a review, see [7] and references therein). The "bottom-up" method consists in incorporation of phosphorus-bearing molecules PH_3 on a preliminary H passivated Si (001) surface during the molecular-beam-epitaxial growth followed by the decomposition of PH_3 at significantly increased temperature. The alternative "top-down" method is based on incorporation of dopant atoms under the surface of the grown structure using ion implantation, followed by the annealing of radiation damage at increased temperatures. In these methods, the depth distribution of the incorporated donor atoms cannot be controlled to the necessary accuracy. As a result, the vertical distribution of the implanted impurities is rather extended. Meanwhile, small fluctuations in the vertical position of P atoms under the gate is very important to minimize the A-gate voltage error rate [8] because otherwise, each qubit would need its own set of applied voltages and each interacting pair of qubits would need its unique pulse time [9].

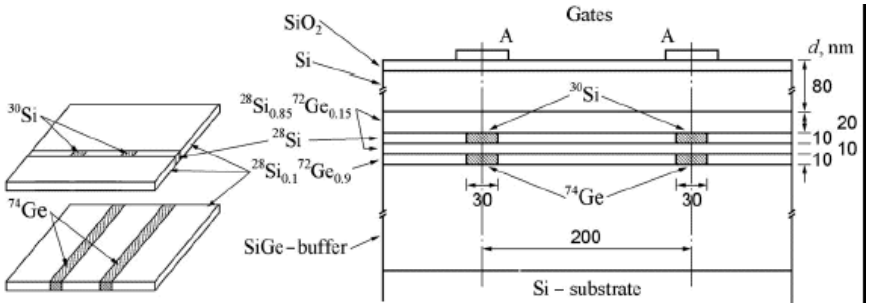

Figure 1: Schematics of the proposed device. After NTD, ^{31}P donors appear only inside the ^{30}Si-spots and underlying ^{74}Ge-strips will be heavily doped with ^{75}As donors. All sizes are shown in nm.

We suggest here a novel technology of the precise placing of P atoms into Si layer. The key point is the growth of the central Si and barrier $Si_{0.85}Ge_{0.15}$ layers from different isotopes: the $Si_{0.85}Ge_{0.15}$ layers from isotopes ^{28}Si and ^{72}Ge and the central Si layer from isotope ^{28}Si with ^{30}Si spots introduced by means of the nano-lithography (Fig. 1). Because different isotopes of Si and Ge are chemically identical, this technology guarantees the high quality of the grown structures.

After preparation, these structures will be irradiated with a neutron flux in a nuclear reactor followed by the fast annealing of radiation damage. The behaviour of different isotopes is different. After capture of a slow (thermal) neutron, a given isotope shifts to the isotope with mass number larger by one. If the isotope thus obtained is stable, this nuclear reaction does not entail doping. However, if the obtained isotope is unstable, it transmutes after half-life time τ to a nucleus of another element with atomic number larger by one in the case of β^-− decay. This method of doping is called NTD - neutron-transmutation doping [10]. In the case of Si, NTD is based on the transmutation of the isotope ^{30}Si:

$$^{30}_{14}\mathrm{Si} + ^{1}_{0}n = ^{31}_{14}\mathrm{Si} \rightarrow \beta^-(\tau = 2.62h) \rightarrow ^{31}_{15}\mathrm{P}.$$

In the isotopically engineered structure, ^{31}P donor atoms will be produced only within ^{30}Si spots, because the isotopes ^{28}Si and ^{72}Ge shift to the stable isotopes ^{29}Si and ^{73}Ge, respectively. Therefore, in the suggested method, the processes of the structure growth and doping are completely separated. The idea to fabricate a basic element for a nuclear spin quantum computer using the isotope engineering of Si and SiGe nanostructures was proposed earlier in [11]. The precise placing of P atoms into a Si matrix by means of the NTD method was suggested in [12, 13].

Let us estimate the feasibility of the proposed method. We consider a ^{30}Si spot of area $S = 30{\times}30$ nm $\approx 10^{-11}$ cm^2, thickness d =10 nm with a distance of 200 nm between spots (Fig. 1). The "buried" distance to the structure surface is halved, 100 nm, which is needed to protect against cross-links and to ensure the influence of the A-gate voltage on the corresponding underlying qubit only. In the proposed method of incorporation of P into Si, the vertical accuracy of the location of P donors is determined by the thickness of the ^{30}Si spot (10 nm) with respect to the distance to the A-gate (100 nm). Indeed, the irradiation of samples by thermal neutrons occurs at room temperatures where the introduced P atoms are immobile. The irradiation is followed by the annealing of radiation damage at higher temperatures (700°C). During the short annealing time (1 hour), impurities cannot diffuse far from the transmutation place; the diffusion length does not exceed 1–2 nm. As a result, the proposed method will provide an almost equal burying depth of P atoms with a controlled accuracy (about 10 % in our example). The number of transmutation events is $\widetilde{N}(^{31}\mathrm{P}) = \widetilde{N}(^{30}\mathrm{Si})\sigma^{30}\Phi$, where $\widetilde{N}$ is the number of atoms, σ is the cross-section of the thermal neutron capture for given isotope ($\sigma^{30} \approx 0.11{\cdot}10^{-24}$ cm^2), $\Phi = \varphi t$ is the integral neutron flux (φ is the intensity of the thermal neutron flux and t is the time

of irradiation). To achieve $\widetilde{N}(^{31}\mathrm{P}) = 1$ for the chosen ^{30}Si spot geometry, $\Phi \approx 2 \cdot 10^{19}$ neutron/cm^2 which corresponds to the reasonable irradiation time $t \approx 2 \cdot 10^5$ s ≈ 56 hrs.

3 Qubit certification

An unavoidable peculiarity of the NTD is the casual character of the neutron capture. As a consequence, after NTD, some of ^{30}Si spots will contain no donor atom ("0-spot") and cannot serve therefore as qubits, while some will contain more than one donor atom. The probability P_m to find "0-spot", "1-spot", "2-spot", and so on ($m = 0, 1, 2, ...$), is described by the binomial distribution:

$$P_m = C_D^m p^m (1-p)^{D-m}$$

where C_D^m is the binomial coefficient, $p = N(^{30}\mathrm{Si})\ \sigma^{30} d$ is the probability for the neutron to be captured in a layer of thickness d, $D = \Phi S$ is the dimensionless dose of irradiation.

The best candidates for qubits are "1-spots", while spots having more than one donor could also be considered as qubits after corresponding theoretical investigation. Only spots without donors ("0-spots") are obviously non-qubits. Using the above expression, one can calculate that the maximal portion of "1-spots" is 37 % at $\Phi^* = pD = 1$. In this case, the portion of non-qubit is also about 37 %. If "2-spots" will be considered as possible qubits, the optimal integral dose will correspond to $\Phi^* = 2$. In this case, the fraction of non-qubits decreases down to 14 %.

To determine the number of donors in each spot, we propose to use narrow source-drain (SD) channels fabricated beneath each donor position (Fig. 1). If the given spot contains one donor, it will form (together with the underlying SD channel and overlying A-gate) a flash-memory field-effect transistor (FET) with the qubit donor acting as a "floating gate". The donor electron is separated from the SD channel and A-gate by the $Si_{0.85}Ge_{0.15}$ barriers of about 10 nm width and 100 meV height [5] which are used for the electron confinement. However, a pulse of relatively strong voltage applied between the A-gate and SD channel will tilt the barriers leading to the abrupt electron transfer and donor ionization at a threshold voltage [14]. An electric field of the positively-charged donor ion located only 10 nm from the narrow SD channel will shift the FET cutoff voltage at the value of about 10 mV, which is easy to observe [15]. If there are two or more donors in the given spot, the cutoff shift will be even larger. If there is no donor underneath the given gate, the shift will not be observed.

4 Source-drain channels fabrication

We suggest a method for the fabrication and the proper alignment of the SD channels with respect to the position of ^{31}P qubits. This method is also based on isotope engineering of a $Si_{1-x}Ge_x$ layer followed by NTD. We propose to make the underlying $Si_{1-x}Ge_x$ layer from a composition close to Ge (say, $Si_{0.1}Ge_{0.9}$) using isotopes ^{28}Si and ^{72}Ge, followed by the fabrication of 30 nm-width strips where ^{72}Ge is replaced by ^{74}Ge (Fig. 1). After NTD, these ^{74}Ge-strips will be doped by As donors through the following nuclear reaction:

$$^{74}_{32}\mathrm{Ge} + ^{1}_{0}n = ^{75}_{32}\mathrm{Ge} \rightarrow \beta^{-}(\tau = 82\,\mathrm{min}) \rightarrow ^{75}_{33}\mathrm{As}$$

Irradiation of the structure with the thermal neutron integral dose $\Phi = 2 \cdot 10^{19}$ cm^{-2} ($\Phi^* = 1$) needed for introducing on average one P donor in each ^{30}Si spot, will also lead to doping of ^{74}Ge-strips with As donors to a high level ($N_{\mathrm{As}} \approx 4.5 \cdot 10^{17}$ cm^{-3}) because of the relatively large $\sigma^{74} = 0.5 \cdot 10^{-24}$ cm^2. This concentration of As exceeds the critical value of the metal–insulator transition for Ge:As [20]. Therefore, NTD-introduced narrow channels will have a metallic-like conductivity and remain conductive down to $T \rightarrow 0$. This is important because nano-FET will operate at low temperatures when donor electrons in ^{31}P-qubits are localized on their donors. For the suggested geometry of the SD channel, with the thickness of the $Si_{0.1}Ge_{0.9}$ layer of about 10 nm, width of the ^{74}Ge-strips of 30 nm and the length about 1 μm, the channel resistance is about 1 MΩ, which is suitable.

5 Two-qubit operation

In this section, we suggest a new mechanism of entanglement for distant qubits. Because direct overlap of wavefunctions for electrons localized on P donors is negligible for distant pairs, we propose another principle of coupling based on the placement of qubits at fixed positions in a quasi-one-dimensional Si nanowire and using the indirect interaction of ^{31}P nuclear spins with spins of electrons localized in the nanowire which we will call hereafter as "1D-electrons". This interaction depends on the amplitude of the wavefunction of the "1D-electron" estimated at the position of the given donor nucleus $\Psi_n(r_i)$ and can be controlled by the change in the number of "1D-electrons" N in the wire.

At $N = 0$, the interqubit coupling is totally suppressed, each ^{31}P nuclear spin interact only with its own donor electron. This situation is analoguous to that one suggested in the Kane proposal [5] and therefore all single-qubit

operations and estimates of the decoherence time are valid also in our case. The difference consists in the method of coupling when a controlled number N of "1D-electrons"is injected into the nanowire. In this case, nuclear spin-qubits will also interact with the spins of "1D-electrons". To estimate the intensity of this interaction we need to calculate $\Psi_n(r_i)$. In the below calculation we believe that the donor potential does not influence the distribution function $\Psi_n(r)$ of "1D-electrons" because it is screened by the donor electron on the relatively short distance of order of $a_{\rm B} \approx 2.5$ nm and $a_{\rm B}$ is small comared with the wire length l.

Let the interqubit distance be $r = 200$ nm, one order of magnitude larger than in the Kane proposal [4]. To realize the coupling between these distant qubits, we suggest fabricating a Si nanowire of length $l = 400$ nm and place P donors at distances $r_1 = (1/4)l$, and $r_2 = (3/4)l$ (see Fig. 2). For $N = 1$ and $N = 3$, the functions $\Psi_n(r)$ belong to the energy levels E_n $(n = 1, 2)$ because in the absence of a magnetic field, each level contains two electrons with opposite spin. The highest amplitude of $\Psi_n(r)$ evaluated at the positions of the nuclear spin qubits r_1 and r_2 is realized at $N = 3$ $(n = 2)$. In this case, the interqubit coupling is maximal.

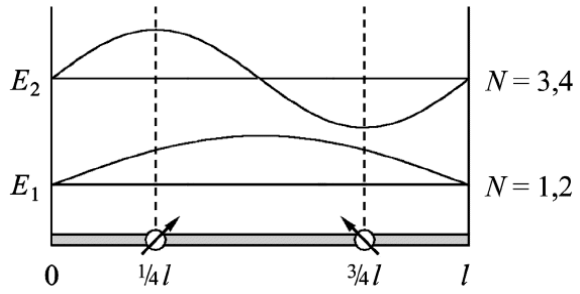

Figure 2: Spatial distribution of electron wave functions for N electrons in a quantum wire of the length l.

To calculate the coefficient of the hyperfine interaction between nuclear and electron spins, we consider, following [22], a system consisting of electrons confined by a potential $V(\vec{r})$ and two nuclear spins. We suppose that the nuclear spins are located far enough from each other so that the direct nuclear spin interaction is negligible. The contact hyperfine interaction between electrons and nuclear spins leads to an indirect nuclear spin interaction. Let the quantum wire have finite length l in the x-direction with the two nuclear spins located at $\vec{r}_1$ and $\vec{r}_2$ in a magnetic field $\mathbf{H}$ directed in the

z direction. The Hamiltonian of the system is given by

$$\begin{aligned} H &= H_0 + H_1 = \frac{1}{2m_e}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)^2 + V(\vec{r}) \\ &\quad -2g\mu_B\boldsymbol{\sigma}\mathbf{H} + \frac{8\pi}{3}\mu_B\gamma_n\hbar\mathbf{I}_1\boldsymbol{\sigma}\delta(\vec{r}-\vec{r}_1) \\ &\quad +\frac{8\pi}{3}\mu_B\gamma_n\hbar\mathbf{I}_2\boldsymbol{\sigma}\delta(\vec{r}-\vec{r}_2) \end{aligned} \tag{1}$$

where H_0 is the Hamiltonian of the electron in the mesoscopic structure in the magnetic field, $H_1 = H_1^{(1)} + H_1^{(2)}$ is the contact hyperfine interaction, m_e is the electron mass, $\mathbf{A}$ is the magnetic-field potential, μ_B is the Bohr magneton, γ_n is the nuclear gyromagnetic ratio, $\mathbf{I}_{1,2}$ and $\boldsymbol{\sigma}$ are nuclear and electron spins, and $\vec{r}_{1,2}$ is radius vector of the nucleus.

The effective nuclear spin interaction energy calculated by second-order perturbation theory is [23]:

$$E = \sum_{E_i,E_f} \frac{\left\langle \Psi_i \left| H_1^{(1)} \right| \Psi_f \right\rangle \left\langle \Psi_f \left| H_1^{(2)} \right| \Psi_i \right\rangle}{E_f - E_i} f_i(1-f_f) + c.c. \tag{2}$$

Here, Ψ_i and E_i are the eigenfunctions and eigenvalues of H_0, and $f_{i,f}$ is the electron distribution function in the initial and final states. We will use expression (2) to find the effective interaction between nuclear spins.

We suppose that the transverse dimensions of the quantum wire are much smaller than its length and the cyclotron orbit of the electron. The confining potential is $V(x,y,z) = V(x) - V_0\delta(y)\delta(z)$, where $V(x) = 0$ if $0 \leqslant x \leqslant l$, and $V(x) = \infty$ otherwise.

The wave function should satisfy the following boundary condition: $\Psi_n(0) = \Psi_n(l) = 0$. The solution has the form

$$\begin{aligned} \Psi_{m,s=\pm} &= \sqrt{\frac{4}{\pi l\delta y\delta z}}\left(\begin{pmatrix}1\\0\end{pmatrix},\begin{pmatrix}0\\1\end{pmatrix}\right)\sin\left(\frac{n\pi x}{l}\right) \\ &\quad \times\exp\left(-\frac{y^2}{\delta y^2}\right)\exp\left(-\frac{z^2}{\delta z^2}\right), \end{aligned} \tag{3}$$

$$E_{n,s=\pm} = \frac{\hbar^2\pi^2}{2m_e l^2}n^2 \mp g\mu_B H, \tag{4}$$

where δy and δz are the transverse dimensions of the electron wave function.

Let us consider the problem at $T = 0$. In this case the electron distribution function f is 1 for the filled states and 0 for the empty states. Inserting

this wave function into Eq. (2) and assuming that the Zeeman splitting energy in (4) is much less than the energy gap between levels with different n, one obtains the following expression for the nuclear spin interaction constant A [22]:

$$A = \left(\frac{32\mu_B\gamma_n\hbar}{3l\delta y\delta z}\right)^2 \frac{\sin^2\left[\frac{N+1}{2}\pi(r_1/l)\right]\sin^2\left[\frac{N+1}{2}\pi(r_2/l)\right]}{g\mu_B H} \qquad (5)$$

It is seen, that at $N = 3$, A is maximal for both qubit positions $r_1 = (1/4)l$ and $r_2 = (3/4)l$. Let us estimate the error caused by unavoidable fluctuations in the positions of nuclear spins in the wire. In our device, the size of ^{30}Si-spot is 30 nm. Therefore, one can expect that the position of NTD-introduced P donor will fluctuate around the central point within ± 15 nm, which is much less than the total wire length $l = 400$ nm. In our model, the interqubit coupling is realized in the case when the wave function of "1D-electron" $\Psi(r)$ has the maximal value at places of the qubit location, where the space derivative $d\Psi/dx$ is close to zero. This makes the coupling insensitive to the form of distribution function and to small fluctuations in the qubit positions.

Thus, the above consideration shows that the indirect coupling is maximal at $N = 3$, while at $N = 0$, the interqubit coupling is totally suppressed. This means that in our model, the entanglement between two distant qubit can be effectively controlled by the proper variation of N.

6 Scalability

Scalability is the one of the most important requirements of the quantum computer proposals [1]. We suggest below the schematics of the device architecture (Fig. 3) which satisfy the scalability requirements. It is worth mentioning that the above method of coupling opens a way to avoid the problem connected with the break in the one-dimensional array of qubits. This problem is inevitable in all proposed technologies. In the method of coupling based on the direct overlap of electron wave functions [4, 6], this requirement is crucial because any break in the one-dimensional array of qubits stops the entanglement along the array and make quantum computation impossible. In our model, entanglement can exist even in the unlikely case of two or more breaks in the qubit array one after another, because indirect coupling can passing over wrong sites by the proper choice of the nanowire length l and the number of electrons N in the wire.

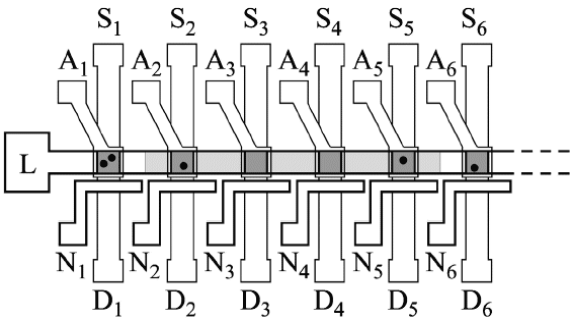

Figure 3: Schematics of a ^{28}Si nanowire L with an array of ^{30}Si spots (qubits and non-qubits after NTD). Each spot is supplied by overlying A-gate, underlying SD-channel and lateral N-gate. This device architecture allows to realize an indirect coupling between any distant qubits (see text).

Figure 3 shows the schematics of the device architecture which allows one to vary l and N. The device consists of a ^{28}Si nanowire with an array of ^{30}Si spots. Each spot is supplied by the overlying A-gate, the underlying SD-shannel and the lateral N-gate. After NTD, P donors will appear in most of the spots (which transforms these spots into qubits) and not appear in other spots (non-qubits). This situation is shown schematically in Fig. 4 where one assume that the spots 3 and 4 are non-qubits ("0-spots") and one need to provide coupling between qubits 2 and 5. For this purpose, it is necessary to connect the gates N_2,N_3,N_4 and N_5. The negative voltage applied between other N-gates and the wire contact L will lead to pressing-out "1D-electrons" from all corresponding areas and formation of the nanowire with $l = 800$ nm between the sites 2 and 5 only (shown in grey in Fig. 3). The coupling between qubits 2 and 5 will be realized via injection in the wire of the necessary number of electrons N, using the positive voltage applied to the gates N_2–N_5. In this particular example, the maximal coupling will be realized at $N = 7$, while at $N = 0$, the coupling will be totaly suppresed.

This paper is devoted to the memory of Israel Vagner and his remarkable contribution to the field of quantum information processing.

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