

Isotopically engineered Si and Ge for spintronics and quantum computation

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ABSTRACT

Si, Ge as well as SiGe structures are the promising materials for spintronics and quantum computation due to the fact that in both crystals only one isotope (^{29}Si and ^{73}Ge) has nuclear spin. As a result, isotope engineering of Si and Ge permits to control the density of nuclear spins and vary the spin coherence time, a crucial parameter in spintronics. In the first part we discuss the NMR study of nuclear spin decoherence in Ge single crystals with different abundance of the ^{73}Ge isotope. It was observed that the slow component of the dephasing process is elongated with depletion of Ge crystal with isotope ^{73}Ge . The second part is devoted to the development of the Kane's model of nuclear spin-based quantum computer, which uses the nuclear spin of ^{31}P impurity atoms in a ^{28}Si matrix as quantum bits (qubits). We discuss a new method of placing ^{31}P atoms in a ^{28}Si based on neutron-transmutation-doping of isotopically engineered Si and Ge. In the proposed structure, interqubit coupling is due to indirect hyperfine interaction of ^{31}P nuclear spins with electrons localized in a ^{28}Si quasi-one-dimensional nanowire, which allows one to control the coupling between distant qubits.

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1. Introduction

Semiconductor-based architectures are quite realistic in constructing the large-scale devices for spintronics and quantum computing (QC) owing to the well-developed semiconductor technology. Among the different QC concepts, nuclear spins are considered to be the ideal quantum bits (qubits) embodied in semiconductor crystals, particularly in Si and Ge. The choice of Si and Ge is determined by the fact that in both these crystals only one isotope (^{29}Si among three stable Si isotopes and ^{73}Ge among five stable Ge isotopes) has nuclear spin, and therefore isotope engineering of Si and Ge permits to control the density of nuclear spins and vary the spin coherence time T_2 , a crucial parameter in spintronics and QC where electron spin or nuclear spin is used as a memory cell and as a qubit [1–3].

The most developed model of the nuclear spin quantum computer is the Kane suggestion [1] to use a precisely located array of phosphorous donors introduced into Si. In this proposal, the nuclear spin $\frac{1}{2}$ of ^{31}P is used as a qubit, while a donor electron together with an overlying gate separated from the donor by a SiO_2 or $\text{Si}_{0.85}\text{Ge}_{0.15}$ barrier, provides single-qubit operation using an external magnetic field and pulses of radio-frequency radiation. In the model proposed for QC based on the electron spin as a qubit [2], different $\text{Si}_{1-x}\text{Ge}_x$ layers are used for modulation of the effective mass and electron spin g -factor. Therefore, Ge along with Si is also involved in different QC architectures. Meanwhile, till

recently, the nuclear spin coherence time T_2 was studied mostly in Si [4,5].

2. Nuclear spin decoherence time in Ge

The ^{73}Ge nuclear spin decoherence was studied in Ref. [6], by means of the nuclear magnetic resonance (NMR) measurements. The NMR signal was measured in Ge crystals with different abundance of the ^{73}Ge isotope. It was observed that nuclear spin decoherence is a double-exponential process characterized by two values T_{21} and T_{22} , and that the deviation from the single exponential decay is more pronounced in the more spin-diluted sample, producing long-lived echoes (Fig. 1).

For natural Ge (7.76% of isotope ^{73}Ge) when the external magnetic field is oriented along the [111] axis, the values of T_{21} and T_{22} are 5.8 and 15.8 ms, correspondingly. In the case of isotopically engineered Ge with 1% abundance of ^{73}Ge isotope, $T_{21} = 1.8$ ms and $T_{22} = 185$ ms. The significant increase of T_{22} with the reduction of ^{73}Ge abundance shows that the long-lived echoes are caused by dipole–dipole interaction, reflecting the fundamental decoherence process in the spin system. The fast decay at the beginning of the echo envelope is assumed to be mainly caused by the quadrupole interaction. Our experimental findings were supported by the theoretical calculations of the Hahn and solid echo decays in Ge crystals [6]. One of the main goals in spintronics and spin-based quantum computing is elongation of decoherence time T_2 . To do this, one should prepare spin-diluted crystals in order to reduce dipole–dipole interactions. Nowadays,

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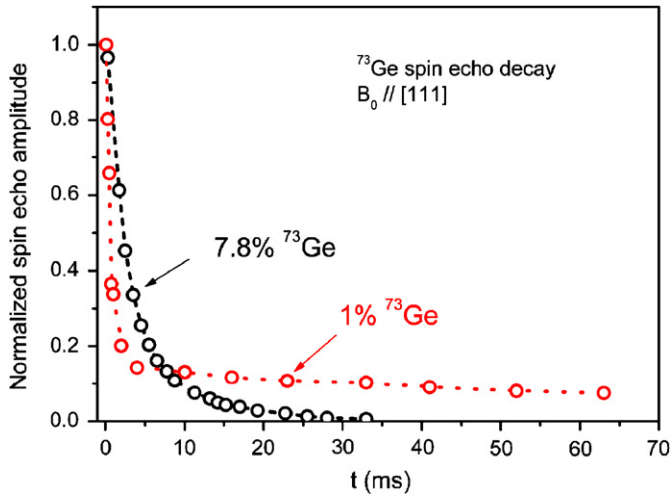


Fig. 1. ^{73}Ge spin echo amplitude decay in Ge single crystal with natural abundance of ^{73}Ge isotope (7.8%) and in isotopically engineered sample with 1% of ^{73}Ge .

semiconductor technology allows successful isotopic engineering and growing the pure monoisotopic ^{70}Ge crystal enriched up to the level of 99.99%, which means that the content of ^{73}Ge isotope is less than 0.01% [7]. Our findings, presented in Ref. [6], show that in such a crystal decoherence time T_2 would be elongated up to ~ 20 s, which is quite an encouraging result for application of this material in SiGe structures suggested in proposals for experimental realization of a nuclear spin-based quantum computers (NSQC).

3. Nuclear spin quantum computer

The most developed model of NSQC is the Kane suggestion [1] to use a precisely located array of phosphorous donors introduced into Si. In this proposal, the nuclear spin $\frac{1}{2}$ 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 $\text{Si}_{0.85}\text{Ge}_{0.15}$ 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 (Fig. 2). 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 between P atoms must be small (less than 20 nm) to allow overlap.

Experimental realization of the suggested model presents a number of difficulties. In Ref. [9], we focus on two problems: placing single P donors into the Si substrate at a precise depth underneath the barrier and 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.

4. Precise placement of P atoms into Si

The key point of the suggested technology of the precise placing of P atoms into a quasi-one-dimensional Si layer technology is the growth of the central Si and barrier $\text{Si}_{0.85}\text{Ge}_{0.15}$ layers from different isotopes: the SiGe 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. 3). Because

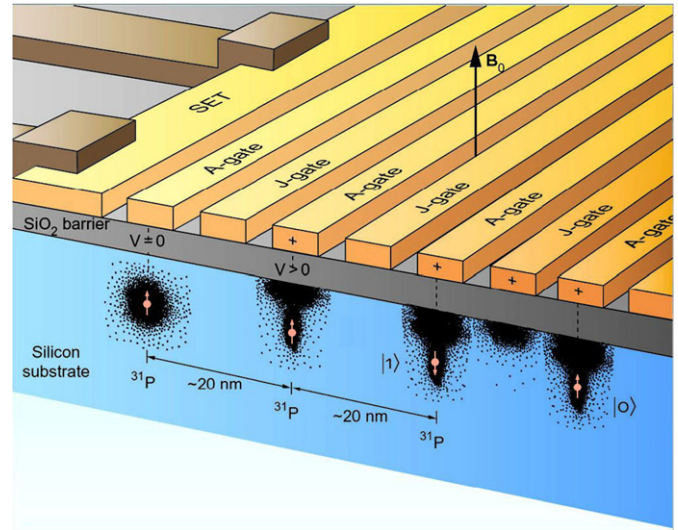
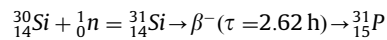


Fig. 2. Schematics of the Kane's model of a silicon-based nuclear spin quantum computer (adopted from Ref. [8]).

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. In this process, called NTD-neutron-transmutation doping [10], the behavior 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 the half-time τ to a nucleus of another element with atomic number larger by one in the case of β^- -decay

NTD of Si is based on the transmutation of the isotope ^{30}Si :



After NTD, ^{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.

5. 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 ($m = 0, 1, 2, \dots$), is described by the Poisson distribution. The best candidates for qubits are "1-spots", whereas spots without donors ("0-spots") are obviously non-qubits. In NTD, the maximal portion of "1-spots" is 37%, while if "2-spots" will also be considered as qubits, the "output" will increase up to 60%.

To determine the number of donors in each spot, we propose to use narrow source-drain (SD) channels fabricated beneath each donor position (Fig. 3). 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 $\text{Si}_{0.85}\text{Ge}_{0.15}$ barriers of about 10–20 nm width and 100 meV height. However, a pulse of relatively strong voltage applied between the A-gate and SD channel will tilt the barriers leading to electron transfer and donor ionization. An electric field of the positively charged donor ion

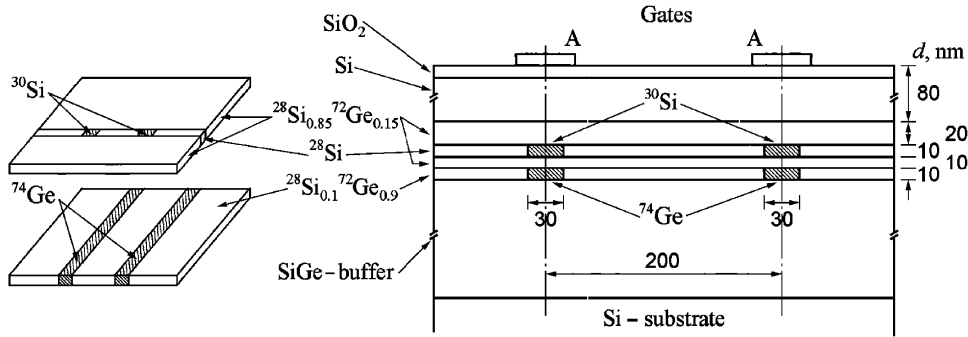


Fig. 3. Schematics of the proposed device. After NTD, ^{31}P donors appear only inside the ^{30}Si -spots. Underlying ^{74}Ge -strips will be heavily doped with ^{75}As donors. All sizes are shown in nm.

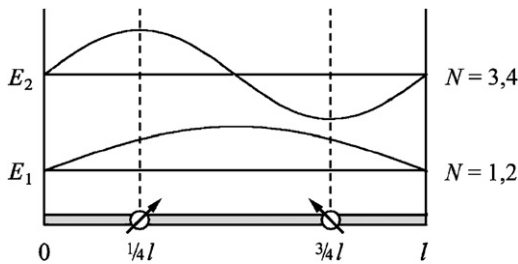


Fig. 4. Spatial distribution of "1D"-electron wave functions for $N = 4$ electrons in a one-dimensional wire of length l .

located only 10 nm from the narrow SD channel will shift the FET cutoff voltage at the value of about a few mV, which is easy to observe. 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.

6. Two-qubit operation

Taking into account that the direct overlap of wave functions for electrons localized on P donors is negligible for distant pairs, another principle of coupling has been proposed in Ref. [11], based on the placement of qubits at fixed positions in a quasi-one-dimensional Si nanowire. In this case, the interqubit coupling will be realized via indirect interaction of ^{31}P nuclear spins with spins of electrons localized in the nanowire, which we will call as "1D"-electrons. This interaction depends on the amplitude of the wave function 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 .

At $N = 0$, the interqubit coupling is totally suppressed, each ^{31}P nuclear spin interact only with its own donor electron. When a controlled number N of "1D"-electrons is injected into the nanowire, nuclear spins will also interact with their spins.

Let the interqubit distance be $r = 200\text{ nm}$, one order of magnitude larger than in the Kane proposal. To realize the coupling between these distant qubits, we suggest fabricating a Si nanowire of length $l = 400\text{ nm}$ and place P donors at distances $r_1 = (1/4)l$, and $r_2 = (3/4)l$ (Fig. 4). Because 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 $N = 3$ or $N = 4$. In this case, the interqubit coupling is maximal.

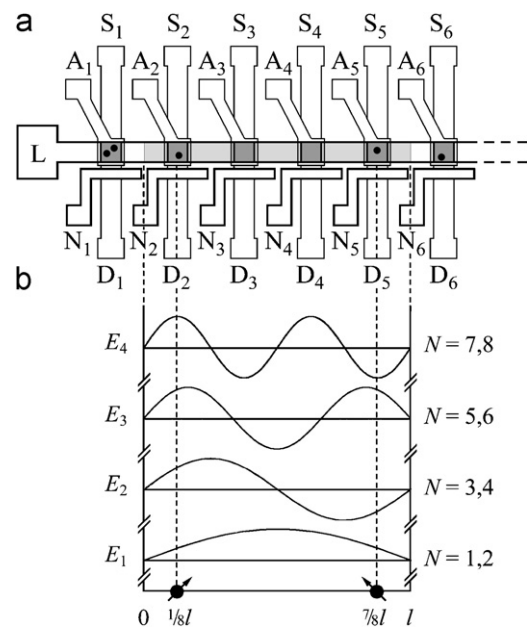


Fig. 5. (a) Schematics of a ^{28}Si nanowire L with an array of ^{30}Si spots (qubits and non-qubits after NTD). Each spot is supplied by overlying A-gate, underlying SD-channel and lateral N-gate. This device architecture allows to realize an indirect coupling between any distant qubits (see text). (b) Spatial distribution of "1D"-electron wave functions for $N = 8$ electrons in a wire of length l obtained by using N-gates.

7. Scalability

The proposed 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 QC architectures.

For example, a situation is shown schematically in Fig. 5a, where 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 together the lateral 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 forming a nanowire with the length $l = 800\text{ nm}$ between the sites 2 and 5 only (shown in gray). 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 when qubits to be coupled are located at $r_1 = (1/8)l$ and $r_2 = (7/8)l$, the maximal coupling will be realized at $N = 7$ or 8 (Fig. 5b), while at $N = 0$, the coupling will be completely suppressed.

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