

Isotopically engineered silicon nanostructures in quantum computation and communication *

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Received 13 October 2003

Abstract

Natural silicon consists of three stable isotopes with atomic mass 28 (92.21%), 29 (4.70%) and 30 (3.09%). To present day, isotopic enrichment of Si was used in electronics for two goals: (i) fabrication of substrates with high level of doping and homogeneous distribution of impurities and (ii) for fabrication of substrates with enhanced heat conduction which allows further chips miniaturization. For the first purpose, enrichment of Si with Si^{30} is used, because after irradiation of a Si ingot by the thermal neutron flux in a nuclear reactor, this isotope transmutes into a phosphorus atom which is a donor impurity in Si. Enrichment of Si with Si^{30} allows one to increase the level of doping up to a factor of 30 with a high homogeneity of the impurity distribution. The second purpose is achieved in Si highly enriched with isotope Si^{28} , because mono-isotopic Si is characterized by enhanced thermal conductivity.

New potential of isotopically engineered Si comes to light because of novel areas of fundamental and applied scientific activity connected with spintronics and a semiconductor-based nuclear spin quantum computer where electron and/or nuclear spins are the objects of manipulation. In this case, control of the abundance of nuclear spins is extremely important. Fortunately, Si allows such a control, because only isotope

*Presented at International Workshop *Frontiers in Science and Technology*.
Holon Academic Institute of Technology, Holon, Israel, 26-27 October 2003

Si^{29} has a non-zero nuclear spin. Therefore, enrichment or depletion of Si with isotope Si^{29} will lead to the creation of a material with a controlled concentration of nuclear spins. Two examples of nano-devices for spintronics and quantum computation, based on isotopically engineered silicon, are discussed.

PACS: 73.20.Dx, 71.70.Ej, 76.60.-k

Development of semiconductor technology is determined by industry requirements. The most exploitable material in the modern electronics and semiconductor industry is Si. More than 90% of semiconductor devices on the market are made from silicon. Two aspects of industrial application caused the development of the isotopic engineering of Si.

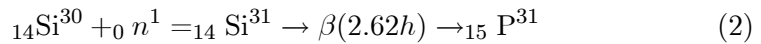
The first one is connected with the problem of homogeneous doping of Si. The tendency in the microelectronic technology is directed to use the Si slices with bigger diameter to prepare more chips in one process. As a result, Si ingots with diameter of 200 and even 300 mm are fabricated now by semiconductor industry. The Si slices with big diameter are used also in fabrication of high power electrical *ac/dc* converters. In both applications, high homogeneity of doping of slices is of crucial importance. In conventional metallurgical methods of doping however, where the impurity is introduced into the melt with subsequent growth of the semiconductor crystal, obtaining a homogeneous distribution of impurities encounters radical difficulties. They are associated with the instabilities in the frontline of crystallization of doped semiconductors and with an unavoidable temperature gradient in the growing ingot between its center and periphery. These difficulties increase dramatically as the ingot diameter increases. Therefore, increase of the ingot diameter leads to increase of heterogeneity in the impurity distribution.

By contrast, neutron transmutation doping (NTD) of Si is characterized by the very high homogeneity in impurity distribution. The NTD method is based on nuclear transformation of isotopes of semiconductor materials following their capture of slow (thermal) neutrons [1, 2]. NTD is achieved by irradiation of semiconductor crystal with a neutron flux in a nuclear reactor. On capturing a neutron, a particular isotope transmutes to another isotope with a mass number larger by one:

$${}_Z N^A \sigma_i \Phi = {}_Z N^{A+1} \quad (1)$$

Here Φ (cm^{-2}) is the integrated flux (dose) of thermal neutrons, σ_i (cm^2) is the thermal-neutron-capture cross section for a given isotope, ${}_Z N^A$ and ${}_Z N^{A+1}$ (cm^{-3}) are concentrations of initial and final reaction products, respectively, Z is the nuclear charge, and A is the mass number of the nucleus.

If the isotope thus obtained, ${}_Z N^{A+1}$, is stable, such nuclear reaction does not entail doping. Of most interest is the case, where the final isotope is unstable. Then after its half-life, this isotope transmutes to a nucleus of another element, with nuclear charge (atomic number) larger by one, ${}_{Z+1} N^{A+1}$ as in the case of β^- decay, or smaller by one, ${}_{Z-1} N^{A+1}$, if the decay occurred by K -capture of the intrinsic electron. One may present here for illustration the reaction producing in silicon a phosphorous donor impurity:



In the case of Si, which consists of three stable isotopes, Si^{28} (abundance 92.2%), Si^{29} (4.7%) and Si^{30} (3.1%), the NTD method has two main advantages over the conventional metallurgical methods of impurity incorporation. First, this is high-precision doping, because the concentration of impurities, introduced at a constant neutron flux, is proportional to irradiation time, which can be controlled with a high accuracy. The second advantage is the high homogeneity of doping [3]. This is provided by the random distribution of isotope Si^{30} in the crystal lattice, the uniformity of the neutron flux (to achieve this, the ingot is rotated about its axis and pulled simultaneously through the reactor active zone during the irradiation), and the small value of σ_i . As a result, high macro-homogeneity of doping was achieved even for ingots with diameter of 200 mm (Fig. 1).

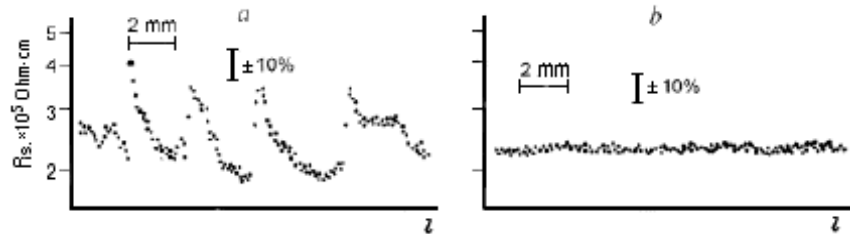


Figure 1: Microdistribution of resistivity in conventionally doped Si (a) and in NTD-Si (b) [3].

However, the NTD method has a limitation, connected with existence of the upper (maximal) level of doping. Indeed, concentration of the phosphorous impurity $N[\text{P}^{31}]$ introduced into Si using NTD method is determined by Eq. (1):

$$N[\text{P}^{31}] = N[\text{Si}]x^{30}\sigma_i\varphi t \quad (3)$$

Here $N[\text{Si}] = 5 \times 10^{22} \text{ cm}^{-3}$ is the density of Si atoms in a lattice, $x^{30} = 0.031$ is the abundance of isotope Si^{30} , $\sigma_i = 0.11 \times 10^{-24} \text{ cm}^2$ is the cross-section for thermal neutron capture by isotope Si^{30} , φ is the thermal neutron flux, t is the time of irradiation. In conventional nuclear reactors, where the value of φ do not exceed usually $5 \times 10^{13} \text{ cm}^{-2} \text{ s}^{-1}$, one month of irradiation corresponds to $2.6 \times 10^6 \text{ s}$, therefore maximal flux is about 10^{20} cm^{-2} and therefore the maximal level of doping is limited by the value of $N[\text{P}^{31}] \approx 10^{16} \text{ cm}^{-3}$. Longer time of irradiation is unwanted because of accumulation of unremovable radiation damages. In this case, the only way to achieve a higher level of doping is the isotopic enrichment of Si with Si^{30} . Taking into account that the abundance of Si^{30} in natural Si is rather small (3.1%), enrichment of Si with Si^{30} can increase the maximal level of NTD doping significantly, up to the factor of 30.

The next field where isotopically engineered Si can be used in electronics is a fabrication of Si substrates with enhanced thermal conductivity. This is an important parameter in fabrication of integrated circuits (IC), because it limits the density of transistors per unit area of substrate. Thermal conductivity of Si is rather high which is an additional reason why this material is widely used in electronics. However, in accordance with the Technology Roadmap for Nanoelectronics [4], it is expected that in 2012 year, the industry will provide IC with over 10^8 transistors per cm^2 for logic and over 10^{10} bits per cm^2 for memory. Such extremely high density of switching elements requires a substrate with enhanced thermal conductivity to take away the emitted heat. In this case, enrichment of Si with one isotope seems to be an effective way to increase the thermal conductivity because variation of masses of different isotopes leads to additional scattering of phonons. Experiments with mono-isotopic Si, enriched with the main isotope Si^{28} up to 99.7-99.896% [5, 6] showed, indeed, an increase of thermal conductivity at room temperature up to 60% in comparison with natural Si (Fig. 2).

New potential of isotopically engineered Si come to light because of novel areas of fundamental and applied scientific activity connected with spintronics and semiconductor-based nuclear spin quantum computer models, where electron and/or nuclear spins are the object of manipulation. In this case, control of the abundance of nuclear spins is extremely important. Even if the electron spin only is considered as a carrier of information, interaction with nuclear spin system determines the electron spin decoherence time. Fortunately, Si allows such a control, because only isotope Si^{29} has non-zero nuclear spin. Therefore, enrichment or depletion of Si with isotope Si^{29} will lead to the creation of a material with either a controlled concentration of nuclear spins, or without nuclear spins at all. One might deliberately vary

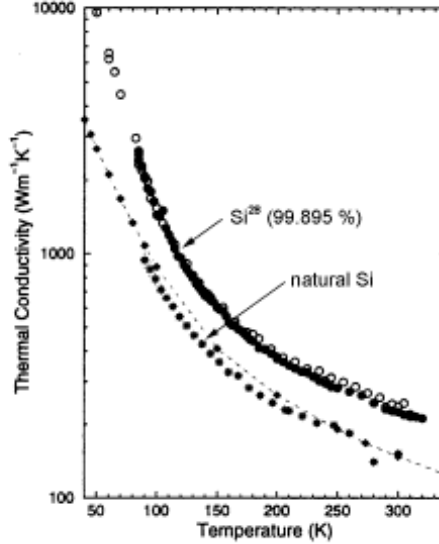


Figure 2: Thermal conductivity data for natural *Si* and isotopically enriched Si^{28} (99.895%) [6].

the isotopic composition to produce layers, wires and dots that could serve as nuclear spin qubits with a controlled number of nuclear spins.

Let us consider an example, where isotopic engineering of Si allows to suggest a basic building block of quantum computation (QC) a technologically viable two-quantum bit (qubit) device for semiconductor-based nuclear spin quantum computer (NSQC) [7]. Nuclear spins are the leading candidates for storing and manipulating QC information because they are well isolated from their environment. Therefore, operations on nuclear spin qubits could have low error rates, and nuclear spin-based data storage elements can have long retention times. The information encoded in the nuclear spin polarization can be detected by an electrical measurement. An ensemble of nuclear spins will be polarized (which means that during this stage, we are concerned with spintronics, rather than QC). The use of isotopically engineered Si, however, enables us to reduce the abundance ratio for non-zero nuclear spin isotopes in a typical size of a quantum dot (10x10 nm) to any small number. The states of the qubit will be encoded in the polarization of nuclear spins in a system of two coupled quantum dots (QDs) fabricated

from a Si/SiGe heterostructure containing a high-mobility two-dimensional electron gas in the quantum Hall effect regime. The nuclear spin polarization will be accomplished via the hyperfine interaction with electron spin system. The same electrons will nondissipatively transfer the polarization between QDs, as well as permit the reading out of the polarization via a magnetoresistance measurement [8 - 10].

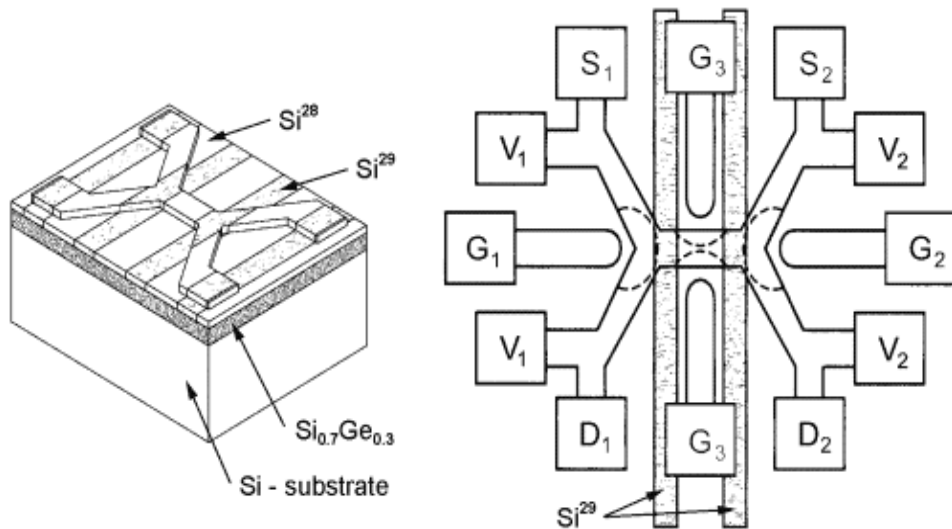


Figure 3: Two nuclear-spin-qubit device made from isotopically engineered Si/SiGe heterostructure

The key feature of the proposed structure is a stripy Si layer which consists of a sequence of strips of non-zero nuclear spin isotope Si²⁹ (or natural Si with 4.7% of Si²⁹) and isotope Si²⁸ with a zero nuclear spin (Fig. 3). Using appropriate negative voltage applied to the gate electrodes G_1 , G_2 and G_3 , one can squeeze out electrons from close-fitting areas of the structure and form a two-qubit system, which consists of two QDs with a few nuclear spins and no nuclear spins in space between dots.

Fabrication of the proposed devices does not present an insurmountable task. Striped Si layer can be obtained using molecular beam epitaxy (MBE) growth on vicinal substrates using multiple Si sources [11]. The only difficulty is the proper alignment of the coupled quantum dot device with respect to the isotopically engineered stripes in the Si quantum well. For this purpose it is suggested to use the nanoscale patterning under the control of atomic force microscope (AFM) [12]. This microscope will be used also for

visualization of the structure steps on the surface of grown heterostructure.

Isotopically enriched Si and Ge compositions are, in principle, available. For example, the properties of highly enriched (99.896%) Si²⁸ were reported in Ref. [6]. In this isotopically enriched Si, the abundance of Si²⁹ and Si³⁰ together is as small as 0.104%. Therefore, the abundance of non-zero nuclear spin isotope Si²⁹ is expected to be about 0.05%. Using this isotopically engineered Si will allow us to achieve only $N = 5$ nuclear spins in the QD of typical size 10x10 nm. The mean distance between nuclear spins will be about 5 nm, which is one order of magnitude larger than the lattice constant in Si. This large distance prevents direct interaction between nuclear spins and make their behavior independent.

We emphasize this fact because existence of interacting (by dipole interactions) N nuclear spins in a given dot leads to highly unwanted multi-qubit gate. In this case, the conduction electron, which entangles two nuclear spins each from a different dot, i.e. exciting one of N nuclear spins in a given dot, will produce a number of excited states of order of $2N$. In contrast, non-interacting N nuclear spins in a given dot form an analog of a single nuclear spin qubit. The only problem is how to detect the quantum computation process which consists in turnover of nuclear spin, if one upturned nuclear spin coexists in a qubit with $N - 1$ nuclear spins which keep the previous spin values. For $N = 5$, this means that the detected signal will be only 20% of the signal from the real single spin qubit system. This is, in principle, solvable problem.

It is easy to show [13] that two nuclear spins, each from another dot, entangled by a conduction electron, represents the logical two-input-two-output SWAP gate, where outputs correspond to unchanged inputs if both inputs are the same and turn over inputs if they are different:

$$\begin{array}{ll} |00\rangle \rightarrow |00\rangle & |11\rangle \rightarrow |11\rangle \\ |01\rangle \rightarrow |10\rangle & |10\rangle \rightarrow |01\rangle \end{array}$$

Let us assume that all N nuclear spins in the 1st QD (dot A) are polarized in "down" direction which corresponds to logical $|0\rangle$, while in the second QD (dot B) all nuclear spins are polarized "up" which corresponds to logical $|1\rangle$. So, the initial state of inputs is $|01\rangle$. Since the Fermi (contact) hyperfine interaction is "selective", the electron-nuclear spin flip-flop process in a system of N independent nuclear spins will take place between a given electron and a one out of N nuclear spins in the dot. Let us assume also that the conduction electron has initially spin "up". The interaction between two nuclear spins via the electron spin will occur as shown in Fig. 4.

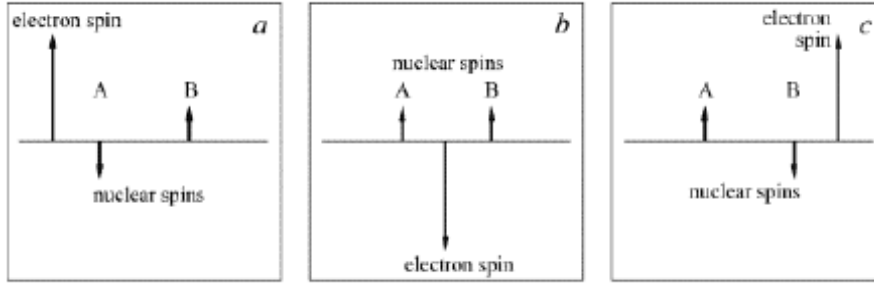


Figure 4: Two-qubit system as a SWAP gate a) Initial state $|01\rangle$: Electron spin is “up”, nuclei are: A is “down” and B is “up”; b) Intermediate state $|11\rangle$ after electron-nuclear spin flip-flop interaction with dot A: electron spin is “down”, nuclei are: A is “up” and B is “up”; c) Final state $|10\rangle$ after following electron-nuclear spin flip-flop interaction with dot B: Electron spin is “up”, nuclei are: A is “up” and B is “down”.

Note, that because the electron Zeeman energy ΔE is more than three orders of magnitude larger than the nuclear Zeeman splitting energy, the intermediate state b) is energetically forbidden and is therefore virtual. The Heisenberg uncertainty relation $\Delta E \Delta t \sim h$ permits this virtual state during the time interval $\Delta t \sim h/\Delta E \sim 10^{-11}$ s. This allows the inter-dot distance up to 10^2 - 10^3 nm which is much more than the maximal inter-dot limit in the proposed technology. One can see also that virtual character of the intermediate state makes impossible the change of nuclear spin direction in both dots if they have the same nuclear spin polarization, never mind what is the distance between dots. Thus, all conditions for the SWAP gate are fulfilled on the quantum level in the proposed two-nuclear spin qubit system.

Enrichment of Si with isotope Si^{30} followed by the neutron-transmutation doping technique (NTD), allows also to suggest a method for preparation of a prototype of an elementary nuclear-spin-qubit embodied in a semiconductor based on fabrication of an isotopically engineered $\text{Si}^{30}/\text{Si}^{28}\text{Ge}$ heterostructure. In such a structure, P atoms will be produced only within Si^{30} strips, because Si^{28} transmutes into stable isotope Si^{29} . Numerical estimations show that to achieve the mean distance of $R \approx 100$ nm between P atoms in a Si^{30} strip of 50×10 nm cross-section, the integrated neutron flux must be about 10^{20} neutrons/cm² which corresponds to the relatively long time (about one month) of irradiation in conventional nuclear reactors. This is due to very small abundance of isotope Si^{30} in the natural composition

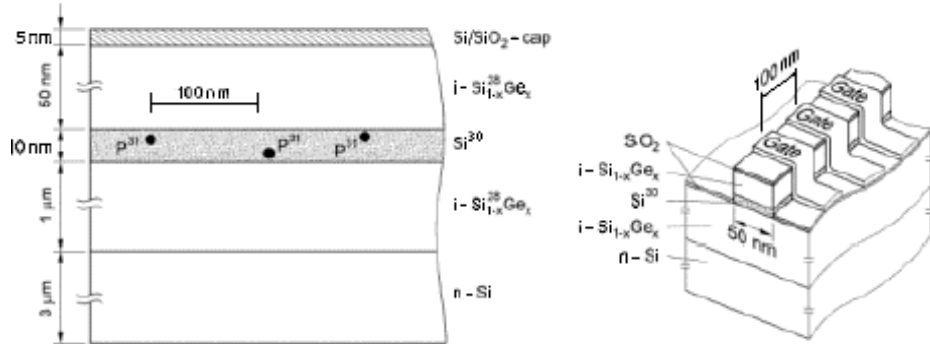


Figure 5: Architecture of the vertical isotopically engineered Si/SiGe heterostructure with P atoms introduced by NTD technique (left) and final Si-nanowire (right) prepared by AFM-assisted lithography with array P atoms under metallic gates.

(3.12%). Enrichment of Si with isotope Si^{30} , for example, up to 30% will reduce the irradiation time down to a few days which is quite reasonable. Large R will allow us to arrange easily the control gates. Entanglement between two separated P nuclear-spin-qubits in such Si wire could be performed by mediation of the conducting electrons. The mean distance R between P atoms will be controlled by the enrichment of Si with isotope Si^{30} and by integral dose of the neutron flux irradiation. Spins associated with P donors will serve as qubits in accordance with the Kane model [14, 15]. Large distance $R \approx 100 \text{ nm}$ will allow to arrange easily metallic gates above P atoms. Entanglement between different qubits will be provided by mediation of conduction electrons in a magnetic field. It is shown theoretically [16] that the hyperfine interaction via the conducting electrons between nuclear spins exhibit sharp maxima as a function of magnetic field and nuclear spin space position. This phenomenon can be used for manipulation of qubits with almost atomic precision.

The information encoded in the nuclear spin polarization could be detected by an electrical measurement of two-electron system using single-electron-transistor [17]. Fig. 5 shows the architecture of the Si/SiGe heterostructure prepared from different isotopes (Si layer is prepared from Si^{30} , but two SiGe layers are prepared from isotope Si^{28}) and the final Si-nanowire with array of P atoms which is expected to serve as qubits in S-MSQC.

Author is thankful to I.D. Vagner, V.I. Safarov and P. Wyder for valuable discussions. This work was financially supported by IST Programme of the Commission of the European Communities, under contract number IST-2000-29686.

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