Monoisotopic Silicon-28 (^{28}Si)

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1. Introduction

1.1 Isotopes

What separates the different isotopes of an element from each other is the number of neutrons in the core of the atom, which also gives the isotopes different mass. The most common example of isotopes is probably the difference between water (H_2O) and heavy water (D_2O), where the latter molecule holds the hydrogen isotope deuterium containing one neutron more than the most common “ordinary” hydrogen atom. In nature silicon is found in three different isotopes, ^{28}Si (~ 92 %), ^{29}Si (~ 5 %), and ^{30}Si (~ 3 %) respectively (Fig. 1).

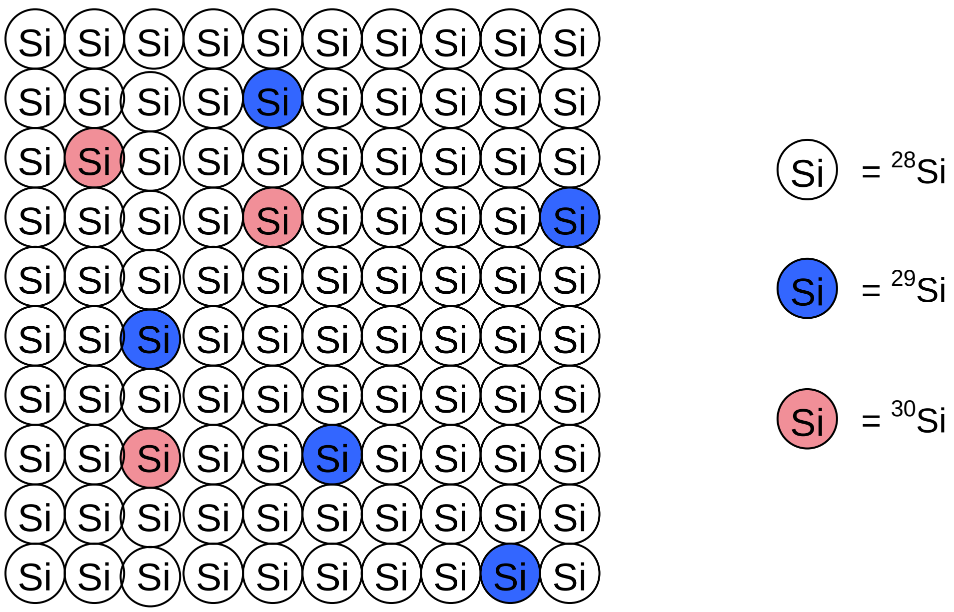


Figure 1. The natural isotope distribution of silicon.

As mentioned above the three silicon isotopes will differ from each other by having a different number of neutrons in the core of the atom. When it comes to the mass of the atoms this leads to ^{28}Si having 3.57 % and 7.14 % less mass than ^{29}Si and ^{30}Si, respectively. This difference in mass will effect vibrations through a silicon crystal containing all three isotopes. The different energy levels of such vibrations are quantified and the vibration modes are called phonons. The phonon vibrations (ω) are related to mass of the atoms (M) in the following way:

$$\omega = M^{-1/2} \tag{1}$$

The phonons play an important role when it comes to transporting heat through a silicon crystal, hence regarding the thermal conductivity of silicon [1–4]. Additionally properties are also effected like the size of the lattice constant, due to the small difference in volume between silicon atoms of different mass [5], and the electronic band gap (by a small change of about 1 meV for silicon [2]).

1.2 Thermal conductivity

In the literature the higher thermal conductivity obtained in monoisotopic silicon as compared to natural silicon has been the main focus. This property can lead to improvements in transistors and microchips based on monoisotopic silicon instead of or in addition to silicon holding the natural isotope distribution. In the literature it seems to be agreement on an improved thermal conductivity of 10 ± 2 % [2–4,6] as a result of reduced electromagnetic noise in monoisotopic silicon as compared to normal silicon, and in ultra pure silicon containing just one isotope (^{28}Si) with very small amounts of isotopic impurities of only the isotope closest in mass (^{29}Si) to the main isotope an even better improvement is probably possible [7]. Reduced electromagnetic noise, in the form of less phonon–phonon and electron–phonon interactions, increases the thermal conductivity of monoisotopic silicon in such a way that the heat generated when electrons move through transistors and microchips is lead faster and more efficiently away in the more perfect crystal lattice created when there is only one isotope present.

A reduction of 5–7 °C in the average temperature of a RF LDMOS power transistor made of ^{28}Si as compared to the same made of ordinary silicon has been measured [6]. A temperature reduction of about 10 °C will more than double the lifetime of such a device, and to give an idea of the costs connected to the generated heat it should be mentioned that the necessary cooling of the servers at the search engines Google and Yahoo contributes more than 35 % of the total operational costs [8].

1.3 Downscaling of electronic devices

Heat generation is of course also an important aspect regarding the downscaling of transistors since the heat is necessarily concentrated on a smaller area.

Another aspect of downscaling is the resulting thinning of the dielectric layer of SiO_2 underneath the “Gate” contact in MOSFET transistors, which increases the risk of electron leakage between the “Gate” and the electron channel through the dielectric SiO_2 layer in between (the so called tunneling effect). When the thickness of the dielectric SiO_2 layer falls below 2 nm tunneling will occur [9], however in a more perfect crystal lattice created by using monoisotopic silicon the interaction between such a layer and the SiO_2 layer will be better and thereby reducing the tunneling effect. Replacing SiO_2 for a dielectric metal oxide, in which the metal can be Hf, Zr, Ce, Sr or even others, will together with the use of monoisotopic silicon have the potential to reduce the tunneling problems even more.

1.4 Speed

The main reason for downscaling of transistors is to increase speed. Regarding the increase of speed in a MOSFET transistor as a result of downscaling in general the following formula applies for the time delay (τ) of a signal through the transistor [10]:

$$\tau = C_{load} \cdot V_{dd} / [\{(W \cdot \mu \cdot \varepsilon)/(L \cdot T_{ox})\} \times (V_{dd} - Vt)^2] \qquad (2)$$

Where C_{load} is stored electrical charge (condensator); V_{dd} is the voltage of the ”Source” in the transistor; W is the width of the ”gate”; L is the length of the ”gate”; μ is the carrier mobility; ε represents a dielectrical constant of the isolating film under the ”gate”; T_{ox} is the thickness of the isolating film under the ”gate”; V_t is the threshold voltage.

We can see from the formula that one way of increasing the speed of such a MOSFET transistor is to reduce the length of the ”Gate” (L), however extremely expensive equipment is required to reduce the length below 70 nm. Another way of increasing the speed is to increase the ”Source” voltage (V_{dd}), but it should be noted that the power consumption of the MOSFET will increase quadratically when this voltage is increased. Reduced thickness of the gate isolating layer (T_{ox}) can also increase the speed, however a reduction below a 1.5 nm thickness is difficult. A gate isolating film with a higher dielectric constant (ε) will increase the speed, but here there are some practical problems to be solved regarding the use of such materials. From the formula we can also deduct that the speed will increase when C_{load} is lowered. It is said [10] that this C_{load} between the source and the drain can be lowered by approximately 1/10 in so called Silicon-On-Insulator (SOI)-type substrates, in which there is a layer of SiO_2 underneath the actual silicon device layer isolating the latter from the rest of the silicon substrate, as compared to ordinary silicon Czokralski wafers. Additionally in such structures the build-up of parasitic capacitance is reduced and combined with an increase in the carrier mobility (μ) as a result of using monoisotopic silicon theoretically a higher speed of MOSFET transistors should be obtained. Another solution lies in using high mobility strained silicon devices like Si/SiGe [11], or even combined Si/SiGeOI devices. However, besides having a beneficial effect on the electron mobility, it is known [12] that both SiGe and SOI based structures have more trouble leading the heat away because of a lower thermal conductivity and the introduction of boundaries (also thermal) in the structure. This might lead to low efficiency in leading away the heat generated as a result of the drain flow of electrons when the transistors are in operation, so called Joule heat, giving rise to functional errors, lower lifetime and reduced speed. It is therefore important having a perfect crystal lattice especially regarding the topography of the surfaces, which otherwise can lead to the generation of local areas with increased Joule heat (hot spots). The best solution in theory would therefore probably be a Si/SiGeOI device based on ^{28}Si, in which also the germanium in the structure should preferably be monoisotopic [10,13]. In a structure like this higher electron mobility should be gained in addition to a parallel reduction of the heat problem

2. Isotopic purification of silicon

2.1 Present challenges

There is a lack of experimental results on aspects regarding monoisotopic silicon other than thermal conductivity. This is because monoisotopic silicon both in the form of solid silicon and silicon containing gases (like $^{28}SiF_4$, $^{28}SiH_4$, $^{28}SiCl_4$, $H^{28}SiCl_3$) are not easily accessible. The reason is probably that the process of purification of such monoisotopic silicon containing gases, and hence the solid monoisotopic silicon, is both demanding and costly. The most common method of isotope purification at present is the isolation of $^{28}SiF_4$ in gas centrifuge separators [14]. Fluorine containing compounds are used because fluorine exists only as one single isotope and thereby the separation is performed solely on the basis of the weight of the silicon isotopes. After the separation the $^{28}SiF_4$ is transformed into $^{28}SiH_4$ via a redox reaction with CaH_2 [15]. This method is used in Russia in the giant centrifuge separators from the cold war period, when they were used for enrichment of uranium related to nuclear weapons production. The process is still restricted because of secrecy and safety regarding the possibility of military use, and additionally very large investments are necessary to be operational. Another method is based on illuminating Si_2F_6 molecules by laser, which generates an isotope selective decomposition into SiH_4 [16,17]. The gain of the latter process is, however, too small regarding mass production and the required equipment is not easily accessible. Other methods based on magnetic mass separation and ion exchange are not capable of mass production of isotopically purified silicon products either. Monoisotopic ^{28}Si is, in other words, very expensive and difficult to produce and thereby not commercially available, which causes the lack of experimental results on possible application for monoisotopic silicon.

2.2 The Isosilicon silicon isotope purification process

The patented Isosilicon process of isotope purification is based on chromatography. This chemical enrichment process uses silane as starting material and is capable of isolating both ^{28}Si, ^{29}Si, and ^{30}Si as their respective silanes.

3. Application of monoisotopic silicon

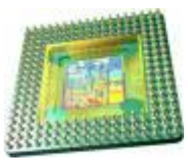
As mentioned above most of the research regarding monoisotopic silicon has been concentrated on thermal conductivity. Isosilicon has ongoing research cooperation with the largest national research institution in Japan (National Institute of Advanced Industrial Science and Technology – AIST) and others to compare monoisotopic silicon to natural silicon regarding other aspects, like electron mobility and carrier lifetime for instance. These are important results to obtain to establish whether the speed of electronic devices and the efficiency of crystalline solar cells, respectively, could be improved by using monoisotopic silicon.

3.1 Solar cells

One problem regarding solar cells is the photo degradation due to boron-oxygen clusters. Their presence leads to shorter carrier lifetime and thereby lowered efficiency. This problem is said to be reduced in solar cells based on monoisotopic ^{28}Si [18] because of their increased thermal conductivity and longer carrier lifetime as compared to solar cells based on normal crystalline silicon. Conversion efficiencies of silicon wafers in which the content of the ^{28}Si isotope was 98 % varied between 21.6–22.6 %, while for the corresponding wafers based on normal silicon efficiencies in the area 20.1–20.9 % was obtained [19]. Cost is, however, very important especially when it comes to solar cells, and the use of monoisotopic material in solar cells depends on an efficient, simple, and cheap process of purification in order to be interesting. The Isosilicon process has the potential to make this possibility a realistic option.

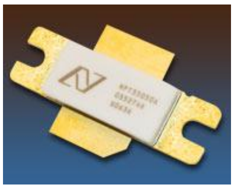
3.2 Mainstream semiconductors

In this category we place products like computer memory, micro-processors, computing- and digital electronics with dissipated powers ranging from < 1W to < 100 W. Monoisotopic silicon in such products will ease the heat dissipation and possibly also increase the speed somewhat.

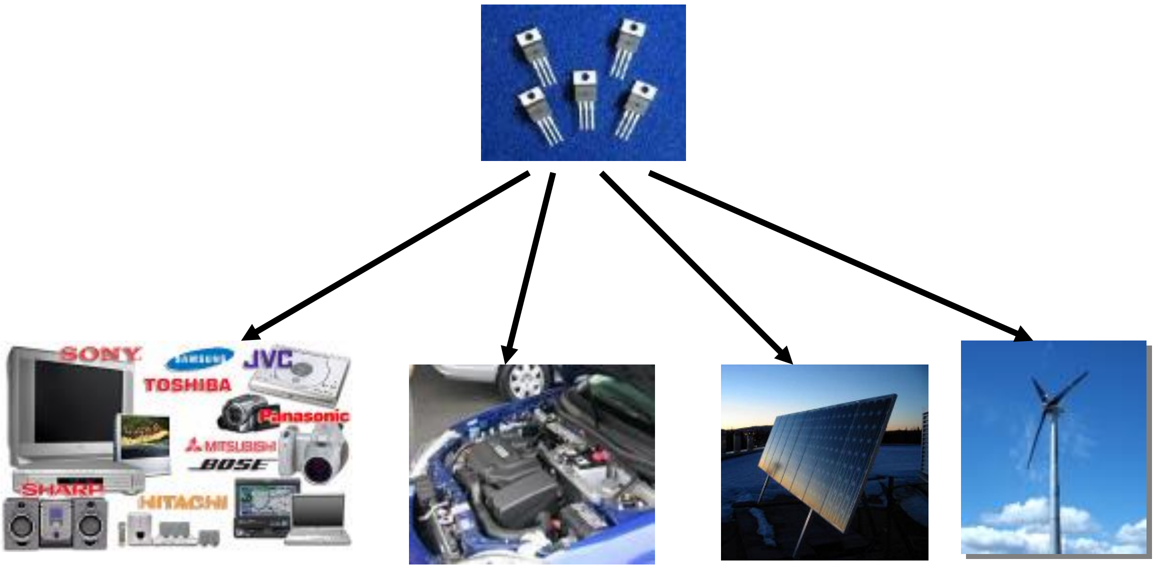
3.3 RF power electronics

High power RF transistors for use in mobile phone base stations are an interesting area regarding use of high thermal conductivity monoistopic silicon because of the large power that needs to be dissipated (100 – 350 W).



3.4 Power electronics

Here we find discrete MOSFETs intended to function in products like for instance ordinary high power (20 W – 1kW) electronic appliances, hybrid cars (5 – 100 kW), parts used in photovoltaic devices to transform direct current into alternating current (100 kW – 1MW) and transistors to function in wind turbines (> 1MW). The improved heat dissipation, giving rise to longer lifetime of the electronic components, in monoisotopic silicon is the most important aspect here as well, but additionally it is possible that the speed of the components could be improved by using isotopically pure material.



3.5 Quantum computers

Quantum computers are based on the principles of the quantum physics properties of atoms and nuclei working together in quantum bits – *qubits*. These qubits can potentially hold exponentially more information than traditional bits. One possible material solution for the representation of the qubits is to use the fact that ^{29}Si has a nuclear spin while ^{28}Si and ^{30}Si don't in all-silicon quantum computers made of ^{29}Si embedded in ^{28}Si [20–22]. Quantum computers have the potential to be much more powerful and fast compared to a normal computer of the same size since a vast number of operations can be performed in parallel. The main challenge regarding the use of silicon isotopes in quantum computers lies in the interaction between the qubits and the environment, that is minimizing the errors caused by the decay from a given quantum state into an incoherent state (so called decoherence).

3.6 Nuclear energy industry

The Pebble bed reactor is a new nuclear reactor concept more suitable for the 21st century regarding safety, efficiency and simplicity. The nuclear fuel is embedded in balls the size of tennis balls as oxides and surrounded by several layers of different forms of graphite as well as silicon carbide (Fig. 2). The silicon carbide layer is implemented to increase the mechanical strength of the capsule at the same time as making the balls fireproof. These properties of silicon carbide could be somewhat weakened if the SiC consists of normal silicon because the ^{30}Si isotope is easily transformed into the unstable ^{31}Si and further into ^{31}P during neutron bombardment. It is therefore better and safer to use layers of ^{28}SiC inside the balls instead.

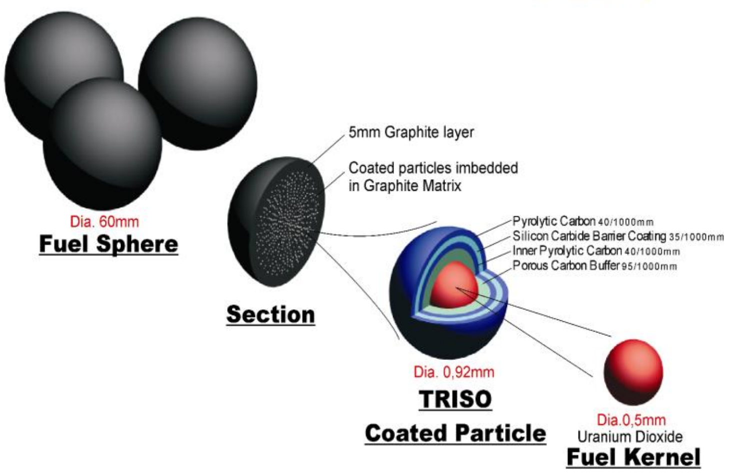


Figure 2. The balls containing nuclear fuel used in pebble bed reactors.

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