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The Enrichment of Silicon Isotope Separation methods: a laser-enhanced deflection approach

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Executive Summary

Quantum computing technology has attracted private funding upwards of US$451 million in 2017-2018 alone. However, obtaining a stable qubit system with minimal noise output remains a significant challenge. Silicon Quantum Dots prove to be a promising method for overcoming the barriers of qubit instability and cost of production. Despite the potential of the technology, silicon isotopic impurities generate background noise that can destabilize electron spin-qubits and lower the performance of quantum computers. Ergo, pure and spin-free silicon for quantum dot design, at reduced costs, is a necessity to minimise decoherence. By building on existing separation techniques, we have designed a NMR inspired technique to obtain isotopically pure ^{28}Si and ^{30}Si. By reducing the cost of silicon isotopic purification, our proposed technique can remarkably contribute to the growing demand for isotopically pure silicon.

Introduction

The prospect of building a functional quantum computer has extended beyond the dreams of optimistic scientists to an immediate goal of the world's leading technology giants.[1] The work by Shor and colleagues in the early 1990s acted as a catalyst for quantum computer development, with the investment of millions of dollars into research for the development of a suite of qubit technologies.[2] As of 2019, a Nature analysis has indicated major private investment to at least 52 quantum technology companies, with $450 million in private funding in 2017-2018 alone.[3] Technology such as trapped ion qubits by start-up company; ionQ, in addition to the superconducting loop technology of tech giants such as IBM, are just some of the promising candidates for functional quantum computers.[1] The remarkable advancements in the field, coupled with the lucrative nature of the industry, have allowed for the remarkable achievement of quantum supremacy. Google scientists were able to develop a supercomputer capable of solving a complex mathematical problem, no standard computer could perform.[4] The large degree of parallelism that these computers offer further pave the way for novel applications such as modelling chemical equations,[5] encryption of data,[6] searching through large data sets[7] and even simulating complex physical systems and phenomena.[8]

Despite the revolutionising potential of quantum computers, significant limitations such as error correction, decoherence and the extreme costs of refrigeration still persist.[9, 10] However, by building on the existing silicon industry, the University of New South Wales are making significant progress towards practical and reliable quantum computing using silicon quantum dots.[10] This system utilizes electron spin resonance (ESR) to enable storage of information by silicon qubits. High purity ^{28}Si and

^{30}Si is necessary to enable optimal functionality and stabilisation of the silicon qubits. This is because ^{29}Si has low coupling and fast flipping nuclear spin which leads to decoherence within the network.[11] Correspondingly, qubits used in silicon quantum dots can be stabilized by using highly enriched ^{28}Si and ^{30}Si due to their lack of a nuclear spin. However, this presents a major challenge, as isotopically purified silicon is extremely expensive and difficult to obtain. The qubits used by Professor Dzurak's research team at UNSW contained 800 ppm residual ^{29}Si atoms.[10] Even at this purity, residual nuclear spins remains the leading cause of decoherence.[9] This presents a novel opportunity to obtain isotopically enriched silicon at a reduced cost. As stated by Dr. Andre Saraiva from the UNSW team, who recently created Silicon Quantum Computing company: "The bottom line is that it is very desirable to lower the residual ^{29}Si by order of magnitude." Thus, to further develop this technology for commercial use, a reliable and cost-effective method of isotopic enrichment is pivotal.

Several industrial techniques for isotopic purification of silicon are currently in existence; however, they present major shortcomings in cost and efficiency. One of the most common is the centrifuge method.[12, 13] The industrial centrifugal separation system generates a centrifugal force to separate isotopes of silicon in a gaseous state. This method separates lighter isotopes of silicon from heavier ones in gaseous silicon tetrafluoride SiF_4. Since natural silicon has three isotopes, the centrifuge repeated separations method is undertaken in successive stages to separate ^{29}Si, arranged in a cascade.[13] This cascade consisted of 230 centrifuges, which was seen as the most productive and efficient method. However, the large number of centrifuges contributes significantly to production cost and requires a vast amount of space. Despite production cost, the technique achieves a measured average isotope richness of 99.9928% $^{28}SiF_4$.[10] The enriched silicon is then converted into SiH_4 using CaH_2 at a temperature of ~180°C with a conversion efficiency of 90%. In order to purify the silicon further, a low rectification was done with the deposition of polycrystalline silicon onto rods which were then used in further purification by float zone single crystal growth.[10]

Due to the high costs of Silicon isotopic enrichment posed by the centrifuge method, it is important that alternatives are deliberated in order to gain a holistic overview of the options available in the industry. An area of investigation that has perhaps not received enough attention is enrichment techniques dealing with gaseous derivatives of Silicon. Our solution entails selective targeting of Silane (SiH_4) molecules containing ^{29}Si nuclei, to aid deflection of this isotope within an applied magnetic field. The innovation of this method lies in the artificial enhancement of vaporised silicon through a cost effective and easily implemented method. Despite the purifying potential of the design, a big obstacle to cost effective operation is the need to cool silane to a point where all electrons are in their ground state. Following deflection, collection and further purification, the isotopically enriched silicon will contain Silicon isotopes 28 and 30. These may in turn be used as the foundation for the production of Silicon Quantum dot qubits that are both affordable and accessible, with qubit ESR undisturbed by Silicon 29 isotopes. Given proper testing and implementation, our proposed technique is highly likely to reduce the cost of Silicon isotopic purification which, by extension, can help meet the growing demand for isotopically pure silicon materials. This will open new avenues for further research and development into Silicon Quantum dot computers.

Proposal

Background of the invention

We considered two main industrial based methods of obtaining a metal in a gaseous state. The first method involves the creation of a flowing neutral steam of metal atoms by heating an isotopically mixed sample in a strong vacuum. The increased pressure would reduce the energy required to sublimate the metal by reducing its vapour pressure. The second separation technique involves deflection of metals within gaseous compounds Our original was based on the former and involved obtaining a neutral gaseous state of silicon which will then be passed through a magnetic field. Since ^{29}Si exhibits a nuclear spin moment (Table 1), it will be deflected by the magnetic field, allowing ^{28}Si and ^{30}Si to pass through undeflected. However, upon discussion with Professor Sven Rogge from the University of New South Wales, it was evident that the small magnetic moment of silicon would require enormous magnetic fields to achieve adequate deflection.

Table 1: The nuclear spin and natural abundance of the stable isotopes of silicon

	Spin ($\hbar$)	**Abundance (%)**
Si-28	0	92.23
Si-29	1/2	4.67
Si-30	0	3.1

The widespread use of silane (SiH_4) in industry, coupled to the relatively small magnetic moments of hydrogen makes it an ideal candidate for gaseous isotope separation. Previously, selective photon irradiation of the compound; $U(BD_4)_4$ has allowed for efficient and low-cost isotope separation.[9] Highly enriched silicon 28 can be obtained by implementing a similar technique. Standard methods for separation, such as centrifuge, depend on the isotopes' physics differences, including mass, size, and electric moments. On the other hand, laser separation isotopes rely only on the idea of electromagnetic radiation absorbed by taking advantage of the slight difference in the energy of the transition of different isotopes. This method has the potential to achieve much larger isotope separation factors. Hence, we could possibly achieve a higher degree of enrichment in a single step.

Description of invention

Building on the work of previous studies, we have designed a method for silicon isotopic separation. Our design uses the principle of isotope separation based on the enhancement of magnetic deflection. By altering the electronic state of a metal gas molecule, an induced paramagnetic state will significantly aid deflection. Our apparatus consists of a laser bombardment section, gas feed section, vapour flow section, laser bombardment section, magnetic deflection section, and a collector (Figure 1a). The setup design further incorporates a vacuum chamber that houses the magnets. The low pressure and low temperature environment of the gas feed chamber ensure that electrons within silane are in their ground state. High intensity laser radiation at a narrow bandwidth is then used to selectively excite silane molecules containing the 29Si isotope to their paramagnetic state. This will significantly aid deflection by the gradient magnetic field induced in the separation system. The excitation process requires a laser operating in the high UV frequency to provide the desired photoionisation of the 29Si isotope. Next, the gas stream will flow to the separation system, wherein the excited 29Si isotopes are deflected from the other isotopes and are thus physically separated. Subsequently, the deflection of the 29Si isotopes into a separate separation chamber, provides an enriched output containing purely 28 and 30 isotopes (Figure 1b).

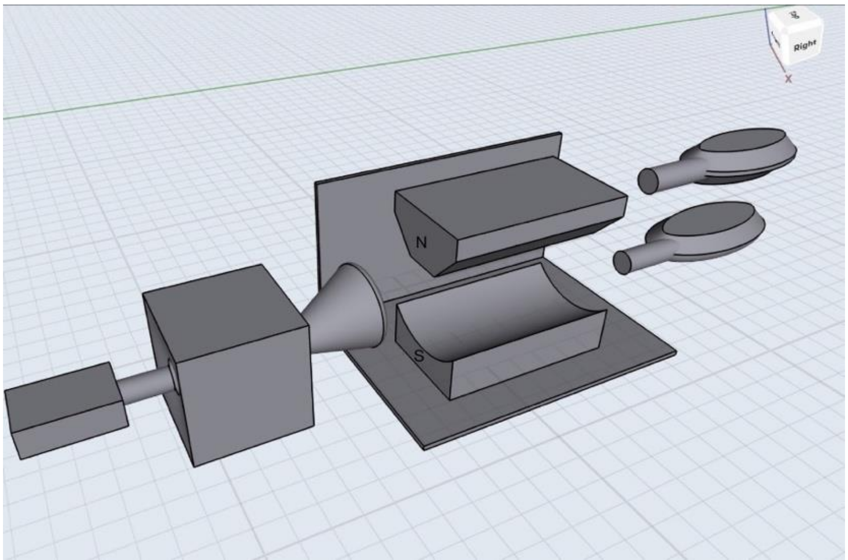

Figure 1 (a): A 3D view of the apparatus.

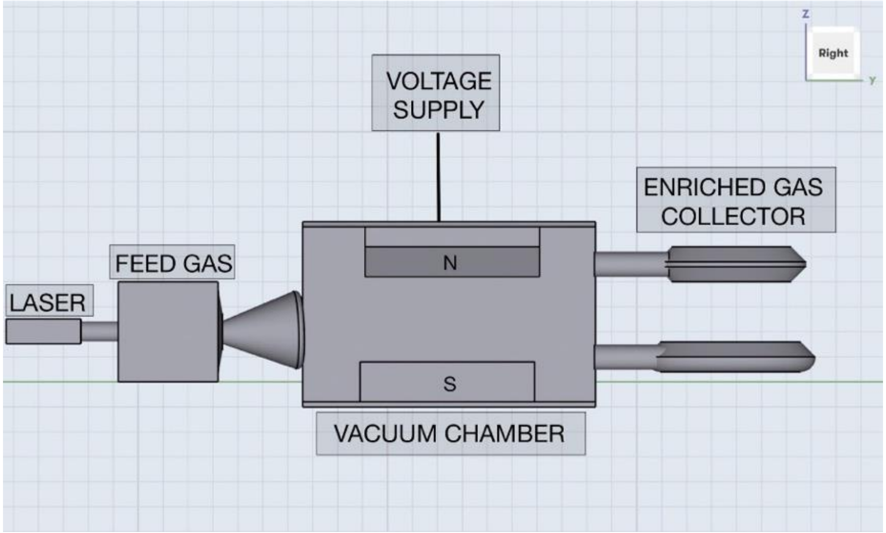

Figure 1 (b): a side view of apparatus

Energy and cost comparison

The operating cost of the centrifuge method is estimated to be the highest among other industrial methods.[14] The cost of the centrifuge method is largely affected by the number of centrifuges used. The method uses 230 centrifuges in a cascade, each centrifuge runs at a frequency of 24Ghz, using 5kW,[15] adding together to accumulate 1150kW. Additional steps were then needed to produce 28Si by itself, adding to the energy needs; thus, furthering expenses. Therefore, both the initial and ongoing costs of 28Si production are substantial. We predict that the cost of our apparatus will mainly be attributed to maintenance, as well as laser, vacuum pump and magnetic field operation, meaning the majority of the financial and energy costs associated with this method are attributed to laser usage. Since the laser contributes significantly to the running cost, alternatives at low cost need to be considered to achieve a more economically viable method. The benefits of our separating apparatus is that more silicon can be produced with less space taken up at an efficient and productive set up. While less space is used up there is still the potential limitation of the running cost being in the range of the centrifuge method.

Limitations and further Research

The three key parameters that necessitate further investigation are the electronic transitions of silane, frequency of laser and the magnetic field strength. Thus, several experiments will need to be conducted to obtain the specific conditions required for a fully functioning apparatus. Our separation technique is based on the principle of electronic excitation. This requires electrons to be in a ground state configuration. As a result, extremely low temperatures are required. This presents a major challenge, as silane exists as a solid below 88.15 K. However, at pressures within the range of $1.59 x 10^{-11}$-$1.96 x 10^{-4}$ bar, silane exists in a gaseous state within a temperature range of 48.15-88.48 K.[16] We propose further studies that examine the ground state configuration of silane at this temperature range. The low vacuum pressure required, as well as the limited knowledge of silane transitions present a limitation to a cost-effective design. This is evident as further studies may indicate that lower temperatures are required for a ground state electron configuration of silane.

At 298K, vacuum ultraviolet spectroscopy (VUV) indicates that the electronic transitions of silane occur in the range of 3.5-165nm.[17] This presents a further challenge as the selective excitation of electrons within silane requires measurements of electronic transitions in the temperature range of 48.15-88.48K. Thus, we suggest a precise experiment aimed at obtaining the electronic transitions of silane at these temperatures. By using an estimated transition at room temperature, we calculated the laser's frequency to be in the range of $8.57 x 10^{16}$-$1.81 x 10^{15}$ Hz. Precise transitions frequencies, as attainable by our suggested experiment, will allow for the determination of the exact laser frequency. We performed rudimentary calculations and found that an electromagnet with a magnetic field of 0.05 T will produce a deflection of 15 cm. However, it is necessary to conduct an additional experiment to confirm the precise magnetic field strength required to produce a deflection for the excited $^{29}SiH_4$ molecules.

Broader significance

The further investigation required to transform our design into a practical and reliable separation technique is justified by the growing market for purified silicon. Despite the implications for quantum computing, the technique can be further applied to the separation of other metal isotopes. This could have far-reaching implications for chemical industries such as nuclear chemistry. A plethora of patents and studies examining the separation of Lithium and Uranium isotopes have resulted in the development of several isotope enrichment techniques. An integration of our design with these techniques, has the potential for industrial-scale application of cost-effective and efficient isotope separation.

A further application could involve the separation of 99MTe and 64Cu isotopes for medical imaging. As of yet, determining the costs associated with the application of our technique proves to be difficult; however future access to laboratory facilities will enable precise cost determination. The possibility of our design not being the most competitive in terms of cost, does not hinder its broader significance. This is because we have confidence in a second market targeted towards governmental research, as our design has the potential for further technological innovation in isotope separation.

Conclusion

Our apparatus holds the potential for a simple, practical and efficient method for silicon isotope separation. The capacity to selectively target and deflect silicon isotopes in a single step process offers several advantages compared to current industrial techniques. The high UV laser frequency and low operation temperatures required are overshadowed by constant advancements in tuneable lasers and refrigeration techniques. We suggest that the next step in achieving a fully functioning apparatus would be to conduct several experiments to indicate the low-temperature electronic transitions of silane. The experiments will allow for precise determination of the required laser frequency. Despite the need for further experiments, we are confident that our design will contribute to meeting growing demand of isotopically pure silicon for high-quality qubits.

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Statement of individual contributions

Corey Gurney (480222110) contributed to the second and third paragraph in the introduction mainly focusing on the third paragraph. This paragraph talks about current methods used in separating silicon. Corey Gurney (480222110) also contributed to the cost and energy comparison paragraph further comparing the centrifuge technique to our proposed technique. In addition to this, editing and writing the executive summary was done by the group.

Hendrik (Malan) Bothma (480352853) contributed towards writing the executive summary. He wrote the first paragraph of the introduction, the first two paragraphs for the background of the invention, the broader significance paragraphs and the conclusion. He further contributed towards writing the limitations and further research paragraphs. Like other members, he helped with the editing and proofreading of the final draft.

Luke Davies (480439453) contributed to the introduction and proposal sections. He planned and wrote a significant portion of the video script and managed the filming and all editing of the film. He also proof-read the report and contributed to team meetings with thoughtful questions pertinent to establishing the direction and outcomes of the different research avenues the group explored.

Twishi Pandit (480334491) contributed to the limitations and proposed further research. They also contributed to part of the second paragraph of the introductions and assisted with the executive summary. They contributed to team meetings by suggesting new ideas as well as ways to adapt to new challenges.

Rowan Alghamdi (490185362) contributed to the executive summary, the second paragraph in the introduction, the invention's distribution, and assisted in the limitation of the technique. Further contributed to the 3D animated design and the setup of the apparatus. Working with the other team members, we contributed toward editing and finalizing the manuscript.

Ali Mahdi (480245278) contributed to the limitations and proposed further research, also assisted with the executive summary. Found the magnitudes of the physical properties of the method such as frequency, energy and an extended analysis to determine the magnetic field which wasn’t included for word count purposes (contact if needed). Proposed new ideas for the physical process of the method Implemented the document into latex in an article format.