Device Modelling and Algorithms Program

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PROGRAM DESCRIPTION

The objectives of the program are to develop comprehensive theoretical descriptions of the Si:P buried dopant charge and spin devices, and all facets of their operation relevant to the short, medium and long-term goals, providing crucial information on device design parameters to the experimental programs. To this end the program has been active in a number of projects including; fundamental solid-state physics of the Si:P donor system, single and coupled qubit operations, the effects of decoherence, large scale simulations of the actual implementation of quantum error correction and algorithms on arrays of qubits, and investigations of new paradigms of quantum computing.

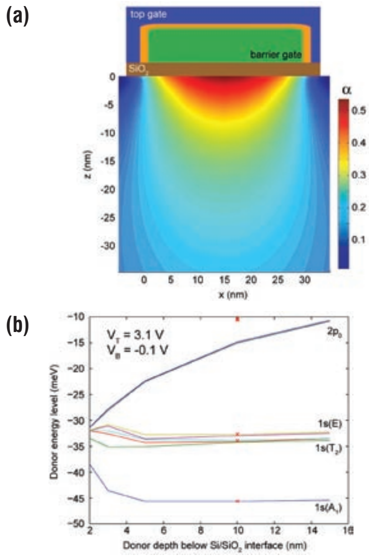

FIGURE 1

(a) TCAD simulation of barrier gate control in a new generation MOS based device. (b) For the same device, donor levels as a function of donor depth.

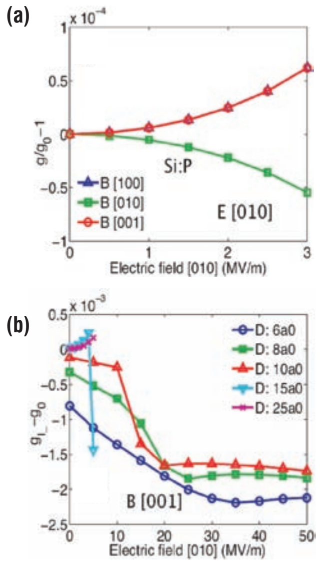

FIGURE 2

(a) Relative change in g-factor of donors with electric fields and parallel or perpendicular magnetic fields. (b) Effects of a nearby interface on the Si:P donor electron g-factor (g-component perpendicular to the field) at various donor depths, D.

1. Overview

In 2008 the Device Modelling Program researchers completed projects ranging from solid-state modelling of silicon devices, implementation issues for fault-tolerant donor-based and optical quantum computing, through to new few-qubit applications. Below is a selection of research highlights.

2. Quantum device simulation

Following the success of the NEMO-TCAD modelling of gated donor FinFET devices [1], researchers have completed an analysis of the donor spectrum as a function of gate bias in the transport MOS devices (Figure 1). These calculations represent the most comprehensive analysis of the orbital effects of gate bias and device structure on single donor levels, and importantly provide valuable clues to the experiments. With the recent experimental successes in fabricating functioning in-plane gated devices, modelling of highly-doped nanostructures and associated incorporated single donor devices is a high priority of the program. While initial Density Functional theory calculations were carried out on the (infinite) delta doped system some time ago, it became apparent that to model the physics of single donor in-plane junctions, new methodology, developed in a separate project, for handling the 1K atom regime need to be engaged.

3. Atomistic treatment of donor spin physics

Through the efforts of centre researchers, the orbital physics of gated donor devices is now well understood. Attention has now been focussed on the associated spin control issues from an atomistic viewpoint. Incorporation of magnetic fields and spin-orbit effects into the tight-binding formalism has been carried out. For the first time the Stark shift of the donor electron g-factor and the anisotropic Zeeman effect has been calculated in the bulk and near an interface (Figure 2) thus probing spin physics in the transition from 3D to 2D confinement.

4. Large scale tight-binding CTAP simulations

The controlled transport of donor electron spins using Coherent Tunnelling Adiabatic Passage (CTAP) has been proposed as a possible transport mechanism in the silicon quantum computer architecture. Following the investigation of CTAP in 1D [2], in a new collaboration with researchers at Sandia National Laboratories large scale tight-binding (NEMO) simulations of a complete CTAP pathway in 3D were carried out. The gated three donor device covered a domain of 60.8 nm × 30.4 nm × 30.4 nm and comprised about 3.5 million Si atoms. The CTAP pathway through the large number of possible gate bias configurations was determined, as shown in Figure 3. These calculations now set the scene for investigations into the level of donor placement precision required for real devices.

5. Topological codes: architectures and thresholds

Surface codes over nearest neighbour qubit arrays offer the promising advantages of topological-like error protection, and high thresholds at the 1% level, without the need for direct physical topological encoding. As such these schemes are interesting as an alternative quantum error correction implementation in the silicon and optical quantum computing framework. We have developed the ability to compute the time-to-failure as a function of code size for a single logical qubit, and hence the memory threshold, using graphical methods for a range of surface code implementations, including the mapping of

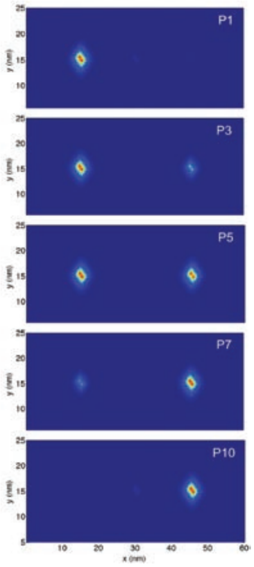

FIGURE 3

Snapshots of the CTAP pathway through bias configuration space showing robust transport of a single electron across a three donor device (left, 15 nm, to right, 45 nm), with minimal occupation of the centre donor (at 30 nm).

such 2D lattices to a bi-linear array. A related development was the development of a scalable photonic quantum computer architecture based on the photonic module [3].

6. Quantum Tomographic Imaging

With the advent of new qubit implementations there is considerable interest in few qubit applications in the lead up to large scale quantum computing. One such application has been developed by Centre researchers – the use of qubits for a new type of imaging mode based on the quantum properties of a qubit probe [4]. Scanning a qubit over a sample and performing on-going quantum tomography, as developed for quantum gate characterization, provides a new window to map not only structure of the sample (in terms of spin distributions), but also the fluctuations occurring within the structure at the nanoscale (Figure 5). The physical implementation of such a scheme would have important applications in nanotechnology and nano-bio systems.

7. Quantum Search with Decoherence

Typically decoherence processes are seen as the bane of quantum information processing, quickly destroying any useful computation or the quantum mechanical aspect of an experiment. However, continuing the theme of tomographic imaging using decoherence we investigated whether decoherence is useful in other contexts. We considered a famous example – the unordered quantum search. We found that an existing method for performing a quantum search (Child's *et al*. measurement-only quantum search [Phys. Rev. A 66, 032314 (2002)]) could be modified so that the quantum search is performed by a specific, tailored, decoherence process. Although the decoherence process is not naturally occurring, it could be generated in a few qubit experiment. Under the right circumstances, it is remarkable that a decoherence process can be used to drive a calculation.

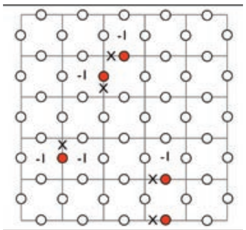

FIGURE 4

Surface code on a 2D qubit lattice. X errors on data qubits are detected by measuring stabilizers around the faces and Z errors are detected by measuring stabilizers around the vertices.

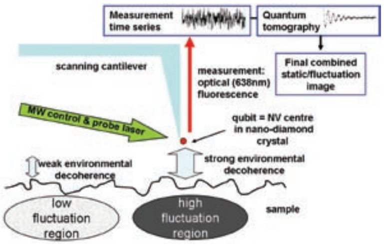

FIGURE 5

Schematic of a quantum tomographic imaging system based on a NV diamond nano-crystal spin qubit.

8. Quantum error correction using message passing

At the heart of quantum error correction (QEC), classical information obtained from measurement can be used to estimate the probability of a logical error in the data qubits. Centre researchers have found that this information at each level can be used to improve higher levels of error correction through a message passing scheme (Figure 7) [5]. Whenever a non-zero syndrome is observed at the physical level, the position in the circuit is flagged at the level above as having an increased likelihood of error on the encoded qubit. These flags can be used to determine the cause of any higher level syndromes more accurately than standard QEC techniques and improve the scaling of concatenation. For two levels of error correction this results in a reduction of the logical failure rate relative to conventional error correction.

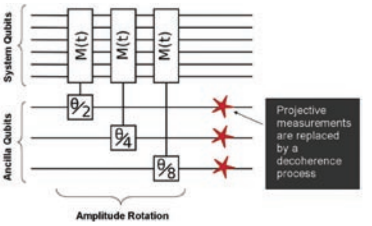

FIGURE 6

Schematic showing a single step of the decoherence based quantum search. This diagram shows coupling from the system to the ancilla (or bath) qubits. Projective measurement called for in the original algorithm is replaced by a continuous decoherence process, indicated here by a star.

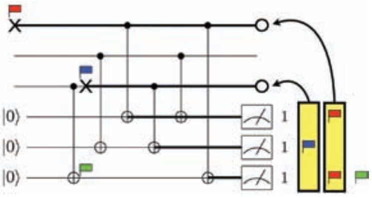

FIGURE 7

Schematic of message passing in quantum error correction. Flags raised by the first level of error correction are tracked through the circuits of the second level of error correction to aid in the diagnosis of level-1 errors. In this example, the blue and red flags match the measured syndrome and are thus identified as being the most likely errors.

9. Publications

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[3] A.M. Stephens, Z.W.E. Evans, S.J. Devitt, A.D. Greentree, A.G. Fowler, W.J. Munro, J.O'Brien, K. Nemoto and L.C.L. Hollenberg, *A deterministic optical quantum computer using photonic modules*, **Physical Review A 78** 032318 (2008).

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