Spin–dependent recombination – an electronic readout mechanism for solid state quantum computers

Christoph Boehme∗, Klaus Lips
Hahn–Meitner–Institut Berlin, Kekuléstr. 5, D-12489 Berlin, Germany

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Abstract

It is shown that coherent spin motion of electron–hole pairs localized in band gap states of silicon can influence charge carrier recombination. Based on this effect, a readout concept for silicon based solid–state spin–quantum computers as proposed by Kane is suggested. The $^{31}\text{P}$ quantum bit (qbit) is connected via hyperfine coupling to the spin of the localized donor electron. When a second localized and singly occupied electronic state with an energy level deep within the band gap or close to the valence edge is in proximity, a gate controlled exchange between the $^{31}\text{P}$ nucleus and the two electronic states can be activated that leaves the donor–deep level pair either unchanged in a $|T^{-}\rangle$-state or shifts it into a singlet state $|S\rangle$. Since the donor deep level transition is spin–dependent, the deep level becomes charged or not, depending on the nuclear spin orientation of the donor nucleus. Thus, the state of the qbit can be read with a sequence of light pulses and photo conductivity measurements.

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∗electronic mail: boehme@hmi.de
1 Introduction

The state of the art of classical computer concepts is rapidly approaching the physical limits as fabrication technology of metal oxide semiconductor logic is minimized to scales where quantum effects determine device properties. While these natural limitations of classical electronics are the dead end for the development of conventional electronics, they open up possibilities for new alternative concepts such as spintronics and quantum computing (QC) [1]. A concept for a silicon based solid state spin–quantum computer as outlined by Kane [2, 3], combines the advantages of conventional semiconductor technology with regard to the high degree to which this technology has been developed and the fundamental concepts of QC, the massive parallel processing of information by coherent quantum states. Kane’s concept takes advantage of the two nuclear–spin energy eigenstates of $^{31}$P-donor nuclei which can be used as well–isolated (long relaxation times) quantum bits (qbits) if they are embedded in a nuclear spin–free crystalline $^{28}$Si matrix. Interaction between these nuclear spin qbits can be controlled by electric fields from charged metal gates above and between the donor atoms which can selectively increase the hyperfine interaction between the localized electron donor states as well as the exchange interaction between electron donor states of different $^{31}$P-atoms [2, 3]. Before an implementation of the silicon based spin–QC is possible, many technological challenges have to be overcome among which the problem of a single spin readout is particularly difficult. In the original proposal [2], the readout of nuclear spin states is done by charge measurements of the qbits’ electronic shell which can contain one or two donor electrons from adjacent $^{31}$P-atoms. Recently, other proposals for the measurement of a single nuclear spin state have been made utilizing single electron transistors [4] or spin–transport in combination with spin refrigeration/spin–readout devices [3].

In this study, a concept is presented, which utilizes spin–dependent charge carrier recombination in silicon for nuclear spin measurements. Electronic transitions between localized, singly occupied paramagnetic band gap states in silicon have known to be spin–dependent since Lepine [5] discovered that electron spin resonant (ESR) changes of such defect states can change recombination rates and therefore photoconductivity. The spin selection rules on these recombination transitions arise from the weakness of spin–orbit coupling in silicon which imposes spin–conservation. Thus, before a transition into a singly occupied state can occur, the two electrons participating have to be in a spin state with singlet content. A model of spin–dependent recombination has been developed by Kaplan et al. [6], who suggested, that spin–dependent recombination processes are always preceded by a selective pair formation of the recombining electrons and holes. Figure 1 illustrates an example of such a process, which was observed by Kanschat et al. [7, 8] in hydrogenated microcrystalline silicon (\(\mu\)c-Si:H). Due to the disorder of this material, shallow trap states exist close to the conduction band which can be singly occupied with excess conduction electrons (CE) at low temperatures. Beside these CE centers, additional dangling bond defect states (db) exist which are excellent recombination centers.
A formation of a spin–pair as described by Kaplan et al. \cite{6} takes place, when a CE state in proximity of a db is occupied. Similar to this example, spin–dependent recombination mechanisms exist in other silicon based materials such as dangling–bond recombination in amorphous silicon \cite{9, 10}, various donor–acceptor and donor radiation–defect recombination pathes in crystalline silicon (c-Si) \cite{11, 12}, in silicon devices \cite{13, 14} and even at c-Si/silicon dioxide interfaces \cite{15} where spin–dependent recombination occurs between stress induced traps and deep interface states.

With regard to silicon QC, the selectiveness of these spin–dependent recombination mechanisms raises the question, whether they could be utilized for a readout of electronic and hence also nuclear spin states, especially since $^{31}\text{P}$ donors are known to show nuclear spin resonance influence on recombination \cite{16}. Precondition for the information readout of coherent spin states with recombination processes is the ability of a given transition to reflect the coherence of the spin states involved, which means the spin–pair states that determine whether a recombination transition takes place or not must not fall into one of the four eigenstates, before a second transition, the actual electronic transfer takes place. This however has never been proven in the past since the experiment used for the detection of all the processes mentioned above (often refered to as electrically detected magnetic resonance, EDMR) is a pure incoherent steady–state magnetic field–sweep experiment, where a constant current of light or electrically injected excess charge carriers is measured while a constant microwave radiation is imposed on the sample. When the magnetic field reaches the resonance of one of the involved centers, a change of the steady state recombination and thus a current change takes place. While EDMR shows that certain

Figure 1: Spin–dependent recombination in the picture of Kaplan et al. for the example of CE-db recombination in µc-Si:H: Since spin–orbit coupling is absent in silicon, the electron in the CE states can only charge the dangling bond, when the CE-db-pair state has singlet content.

![Diagram of spin-dependent recombination](image)
magnetic centers have an influence on recombination, it fails completely to reveal any information about coherence times of the systems involved which are not only the spin–relaxation times of the respective spin centers but also electronic transition times such as recombination or dissociation of the spin pair.

In the following an experiment is presented that shows how coherent spin precession of electrons in localized band gap states can govern recombination rates. Based on this observation we propose an architecture for a recombination based readout of $^{31}$P-qbits.

## 2 Coherent spin motion effects on recombination

Time–domain measurements of spin–dependent recombination (TSR) were carried out on the CE-db mechanism in $\mu$c-Si:H, that is mentioned above. TSR is the electrical detection of pulsed ESR and therefore the time resolved equivalent of EDMR \[17\]. It combines the advantages of EDMR with regard to the selective detection of distinct recombination processes and the advantages of pulsed ESR with regard to its ability to detect coherent spin-motion effects.

The idea of the experiment carried out is to manipulate the steady state of the CE-db pair–ensemble with pulsed ESR on a nanosecond time scale and to observe the transient photocurrent response that is determined by the recombination rate through these centers. Excess charge carriers are generated by a continuous light source. Since singlet states have only short lifetimes, a high density of triplet states is present in the steady state when resonant microwave radiation is absent \[18\].

The orientation of the magnetic moments of $\{T_–\}$–pairs is illustrated in fig. 2 in the rotating frame Bloch–sphere representation \[19\] of the two respective spins contained in the charge car-

Figure 2: The propagation of the CE-db pair ensemble illustrated with Bloch spheres in the rotating frame picture. The three sketches correspond to the steady state, the moment of phase reversal at a time $t = \tau_{180^\circ}$ after the pulse began and the moment of phase recovery $t = 2\tau_{180^\circ}$ for strongly distributed Rabi–frequencies.
rier pairs. If a microwave that is in resonance with the dangling bond and polarized along the $x$–axis is switched on, Rabi–oscillations of the db spins take place. The influence of the microwave pulses on the CE centers is small due to their different resonance frequencies. The Rabi–oscillation of the db spin would lead to an oscillating recombination rate which could be detected as an oscillation of the photocurrent, if the inhomogeneities present in $\mu c$-Si:H did not cause a rapid dephasing of the db ensemble within less than one oscillation period (illustrated in fig. 2). This dephasing is still a coherent process, however, its effect on the recombination rate (strong attenuation of the Rabi induced oscillation) makes it indistinguishable from incoherence. Thus, a rephasing of the ensemble has to be induced, so that incoherence and dephasing becomes distinguishable. As illustrated in fig. 2; a reversal of the direction of spin precession caused by a reversed $B_1$-microwave field causes such a rephasing. The $B_1$–field reversal, done by a microwave phase change that is introduced at an arbitrary time $\tau_{180}$, causes a maximum recovery of the $|T_-\rangle$–density at time $2\tau_{180}$ and hence, a minimum of the recombination takes place. This minimum, which we call a recombination echo will only be detectable, if incoherent processes are not faster than the time scale of the pulse sequence. The detection is a proof of the coherence of the charge carrier pair’s spin motion.

Experimental details with regard to the $\mu c$-Si:H sample and the TSR setup are identical to those of ref. [17] except that the laser intensity was 300mW, the sample temperature $T = 30$K and the intensity of the coherent microwave radiation 500W. The experimental results are displayed in figs. 4 and 3. Note that the detection of fast photocurrent changes in the pA-range with constant offsets in $\mu$A-range is extremely difficult due to noise limitations. The initial decrease of the real–time photocurrent displayed in fig. 4 is therefore due to the rise time of the detection setup. As explained elsewhere [20, 17], the amplitude of the exponential photocurrent relaxation back to the steady state is determined by the coherent spin state prepared during the ns-pulse sequence. Hence, a measurement of the real time signal at a certain time after the rise time versus the pulse length reveals the spin motion during the pulse sequence on a ns-scale. This pulse length dependence, measured at the photocurrent minimum ($t = 19.5\mu$s) after the pulses, is displayed in fig. 3. It clearly displays the photocurrent increase after a sequence of two 100ns long microwave pulses with equal $B_1$-field strength but opposite phase orientations. The width of the echo displayed in fig. 3 turns out to be antiproportional to the $B_1$-field strength which proves the involvement of Rabi–oscillation in the recombination echo effect (not shown here). The two real time transients displayed in fig. 4 are recorded after resonant excitation of the db center. In both cases, the total length and the power of the pulses were identical and only a phase change of 180° was introduced in one case. The smaller amplitude of one transient is solely due to this phase change after 100ns which led to the rephasing of triplet states. An identification of singlet and triplet states with the two binary digits (labeled “1” and “0” for instance) used for information processing allows a direct readout with current measurements.
Figure 3: The amplitude of measured current transients after resonant pulse sequences. After 100ns, the polarization of the microwave field $B_1$ is reversed into its opposite direction, which causes a rephasing after a second period of 100ns. This rephasing after two periods of length $\tau_{180}=100\text{ns}$ is indicated by the increase of the photoconductivity.

3 Spin–dependent recombination and nuclear spin measurements

Based on the observation above, a setup for a recombination readout of Kanes’ silicon based quantum computer is proposed as illustrated in fig. 5. The device proposed consists of a point defect that introduces a deep level paramagnetic state in proximity to the $^{31}\text{P}$-donor which is to be read out, a readout–gate (R-gate), and an additional A-gate above the defect. The latter is only necessary if the defect is induced by a deep level donor with nuclear spin ($I \neq 0$). When the nature and the implementation of the paramagnetic deep level state will be discussed in the following section, it will be refered to as db in this section in consistenc with the dangling bond used for the experimental demonstration discussed above.

The idea behind this setup is to take advantage of Pauli’s principle, similar to the charge–readout proposed by Kane. As long as the R-gate is charged negatively, the wave function overlap between the donor electron of the $^{31}\text{P}$ and the db is small which minimizes a transition probability between the two states and keeps the spin–exchange negligibly small as well. When the R-gate is charged positively, such that the wave function overlap between the $^{31}\text{P}$ and the db is sufficiently large, exchange
Figure 4: Real-time photocurrent transients after resonant microwave excitation of equal length (200ns), equal frequency (db–resonance) and equal intensity (P=500 Watt). The transient where a phase change was introduced after 100ns exhibits a smaller photocurrent quenching due to the higher triplet density among the CE-db pairs. When triplet states represent a binary information “0” and singlet states represent “1”, a current discriminator connected to the sample can read out a spin state electronically.

interaction increases. If this increase is introduced slowly, an adiabatic change of the spin-pairs’ energy eigenstates can take place from an uncoupled product base into a set of singlet and triplet states. At low temperatures ($T \leq 100\,\text{mK}$), the uncoupled pair is polarized in a $|T^-\rangle$-state as long as the coupling is absent. When the exchange is increased slowly, this $|T^-\rangle$-state remains either unchanged or shifts into a $|S\rangle$-state, depending on the orientation of the $^{31}\text{P}$-nucleus (illustrated in fig. 6). Note that in presence of a second nuclear spin at the db-site, the A-gate above this site would have to be charge positively in order to minimize hyperfine coupling. After the R-gate has been “opened” and the electronic pair is in singlet or triplet state, an electronic transition can take place which charges the db; this transition however is possible only when the electronic pair has singlet content in advance and thus, the charging of the db state depends on the nuclear state of the $^{31}\text{P}$ qbit.

The timing and a sketch of the transitions during a readout sequence are displayed in fig. 6. As long as quantum operations on the qbit take place, no light
Figure 5: Illustration of the readout setup. A point defect induces a paramagnetic deep level state (here labeled db) in proximity to the $^{31}\text{P}$ donor. The charge on a readout–gate (R-gate) controls the P-db-exchange interaction. When the P-db-pair is in singlet state after the R-gate is opened and the exchange is present, the P-electron can undergo a transition into the db state which charges the P center positively and the db-center negatively.

is imposed on the sample and the R-gate is charge negatively. When the readout sequence begins at a time $t_0$, the bias of the R-gate is slowly inverted towards a positive voltage. Once exchange coupling is established after a time $\tau_{\text{slope}}$, it remains unchanged until the actual recombination transition has taken place. The time necessary for this transition is of the order of the electronic pair states’s lifetime $\tau_{\text{life}}$, after which the exchange interaction is switched off again. The nuclear spin state of the $^{31}\text{P}$ donor is then coded in the donor and db charge state. A short ($\tau_{\text{flash}}$, ns-Range) and weak (nW-range) laser pulse imposed on the sample will then increase conductivity by the generation of a few pairs of excess electrons and holes. If the donor and the db state are not charged (no transition), a slow decrease of the photoconductivity will follow, which is determined by slow band–band recombination in the ultra pure $^{28}\text{Si}$ bulk. If the two states are charged, a fast decay will take place since charge carriers will be trapped in the charged states. Thus, the level of the photoconductivity a time $\tau_{\text{decay}}$ after the end of the laser pulse will reveal the result of the readout process. Note, that the readout process itself automatically neutralizes the two states such that a new series of operations can take place after its completion.
Figure 6: Adiabatic change of the P-db energy eigenbase. In absence of exchange interaction, the pair remains in product base states. When the exchange is turned on, the states change toward the singlet or triplet states. At low temperatures, the $|T-\rangle$-state is occupied without exchange coupling. Due to hyperfine coupling, the change of this state with increasing exchange interaction is determined by the state of the nuclear spin of the P donor.

4 Challenges of the implementation

The experiments presented above are the motivation for the concept proposed in this study and many other questions will have to be answered experimentally before an actual proof of this concept can be given. The implementation of the singly occupied deep level state will mostly depend on whether it is possible to control its location and whether its charge carrier capture cross sections and the given transition times of the system are fast enough. The dangling bond present in amorphous and microcrystalline silicon would be an ideal system with regard to the latter properties. However, the high disorder in the microcrystalline morphology of silicon makes it a bad choice for QC. Since no process has been established which allows the creation of a single db with A-accuracy at an arbitrary site, a different way of deep level implementation must be chosen.

Various impurities and defects provide singly occupied, paramagnetic deep level donor states in c-Si, some of which are gold, potassium, strontium or chromium [21]. An additional possibility could be interface recombination. Recombination at c-Si/SiO$_2$-interfaces has shown to have spin-dependent paths [15]. Hence, the very same processes which limited the original pure c-Si QC-concept and led to the pro-
Figure 7: Sequential diagram of the readout timing (a) and the corresponding electronic transitions within the energy levels (b). The different steps of the entire readout process are labelled with encircled numbers 1 to 3. At the end of the process at time $t_{read}$, a photocurrent measurement reveals the value of the qbit. For details see text.

A proposal of Si/SiGe-heterostructures [3] could actually be beneficial for a recombination readout mechanism.

Beside the questions for a proper implementation of the deep level center, several other issues remain to be investigated: Due to the necessity of error correction, one of the preconditions for QC is that readout does not destroy the state of the qbit. Therefore, only P-deep level–transitions are possible which leave the $^{31}$P–relaxation unchanged. Important for the feasibility of the recombination readout will also be the question of the overall readout time which should not exceed a lower microsecond range. When the P-deep level transition takes place, the slow relaxation of non–equilibrium polarization at low temperatures could pose a problem due to charged P-deep level–pairs which are neutralized by excess charge carriers produced in excited spin states. The time needed for the relaxation of these states could be very long. However, this problem may be solved by injection of excess carriers by spin–polarized electronic injection instead of light injection. Finally, the question for the one–qbit sensitivity has to be asked: Time–domain measurements of spin–dependent recombination have shown to be sensitive enough to detect the influence of as little as 50 charge carrier pairs, even though the experiment was carried out in the presence of a strong constant photocurrent offset. For the readout as proposed, a measurement without offset could be made and the detection would be even more sensitive. A 2eV laser pulse of 1ns length and 3.2nW intensity produces 10 electron–hole pairs if the internal quantum efficiency is assumed to be 100%. The detection of these 10 charge carrier pairs would require a pA–current measurement on a microsecond scale which does not pose a problem – however, whether the 10% difference between the two readout results caused by the one recombination center
are detectable can only be proven when an implementation of the proposed setup is available.

5 Summary

The demonstration that coherent spin–states of electrons and holes trapped in CE and db states can govern their recombination rate has motivated the idea of a readout mechanism for $^{31}$P qbits in c-Si. A concept, based on a sequence of exchange gating, light pulse and photocurrent measurements was proposed, various implementations suggested and possible limitations and drawbacks discussed.
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