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Broadband electrically detected magnetic resonance using adiabatic pulses

F.M. Hrubesch*, G. Braunbeck, A. Voss, M. Stutzmann, M.S. Brandt

Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

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ABSTRACT

We present a broadband microwave setup for electrically detected magnetic resonance (EDMR) based on microwave antennae with the ability to apply arbitrarily shaped pulses for the excitation of electron spin resonance (ESR) and nuclear magnetic resonance (NMR) of spin ensembles. This setup uses non-resonant stripline structures for on-chip microwave delivery and is demonstrated to work in the frequency range from 4 MHz to 18 GHz. π pulse times of 50 ns and 70 µs for ESR and NMR transitions, respectively, are achieved with as little as 100 mW of microwave or radiofrequency power. The use of adiabatic pulses fully compensates for the microwave magnetic field inhomogeneity of the stripline antennae, as demonstrated with the help of BIR4 unitary rotation pulses driving the ESR transition of neutral phosphorus donors in silicon and the NMR transitions of ionized phosphorus donors as detected by electron nuclear double resonance (ENDOR).

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1. Introduction

Electrically detected magnetic resonance (EDMR) [1] is a versatile method to characterize point defects and charge transport in inorganic and organic semiconductors [2-6]. Due to its high sensitivity it allows for the detection of ensembles with as few as 50 spins in spin-pair-based readout processes [7] and of single electron or nuclear spins when single electron transistors are used for readout [8]. The prototype spin pair investigated in the present paper is formed by an unsaturated paramagnetic silicon dangling bond at the Si/SiO₂ interface between Si and its native surface oxide together with a ³¹P donor electron in close vicinity to the interface [9]. If the spin pair is in a parallel spin configuration, recombination of the electron from the donor to the dangling bond state is Pauli forbidden. Using resonant microwave (mw) excitation the Pauli blockade can be lifted by flipping one of the spins involved which leads to increased recombination and a quenching of the (photo-) current through the sample which in turn can be detected electrically. The characteristic signature of the dangling bond spin is the P_{b0} center with an anisotropic g-factor of $g_{\parallel}=2.0018$ and $g_{\perp}=2.0081$ [10]. The g-factor of the phosphorus donor is $g_P = 1.9985$ with a hyperfine interaction with the ³¹P nucleus of A = 117.53 MHz and a nuclear g-factor $g_n = 2.2601$ [11]. This leads to an overlap of one of the hyperfine-split phosphorus resonances and the dangling bond resonances at X-band frequencies which hampers experiments performed on these resonances.

The use of broadband microwave delivery structures can mitigate e.g. the problems caused by this overlap and allows for multi-frequency or frequency-swept spin resonance experiments which would otherwise require the use of several resonators and multiple cool-down cycles. Broadband microwave striplines have been used successfully for continuous wave (cw) EDMR experiments [12–14] and for pulsed experiments on single spin devices [15,16]. However, in contrast to resonator-based EDMR experiments these structures exhibit significant inhomogeneities of the microwave magnetic field B_1 , which are relevant for pulsed EDMR experiments on ensembles.

Nuclear magnetic resonance (NMR) experiments with surface coils [17–20] and recent experiments on superconducting coplanar waveguide resonators [21], to name but a few, have demonstrated the capability of adiabatic pulses to correct for such B_1 inhomogeneities. Here we show that stripline antenna structures in combination with adiabatic pulses can be very successfully used to excite pulsed EDMR as well as pulsed electrically detected electron nuclear double resonance (ENDOR) employing the same antenna for delivery of electron spin resonance (ESR) and NMR frequencies. In order to use adiabatic or optimum control pulses as discussed e.g. in [22], our broadband setup consists of two arbitrary







^{*} Corresponding author. *E-mail addresses:* florian.hrubesch@wsi.tum.de (F.M. Hrubesch), georg.braunbeck@wsi.tum.de (G. Braunbeck), andrej.voss@wsi.tum.de (A. Voss), stutz@wsi.tum.de (M. Stutzmann), martins.brandt@wsi.tum.de (M.S. Brandt).

waveform generators in combination with a 10 W broadband microwave and a 200 W radiofrequency (rf) amplifier and is able to generate arbitrarily shaped pulses with microwave frequencies between 2 and 18 GHz and radiofrequencies from 1 to 150 MHz with π pulse times as short as 50 ns for a microwave power of 100 mW and 100 µs for a radiofrequency power of 50 mW.

2. Simulation of the stripline short

The optimization of stripline structures for single spin experiments has been extensively covered [16]. The requirements stated there also hold for spin ensembles: The amplitude of the oscillating magnetic field B_1 has to be big enough to yield pulse durations shorter than the spin dephasing time T_2^* of the spins to be studied which is around 60 ns [23] in our test structures due to the interaction with the ²⁹Si nuclear spins present in our samples with natural isotope composition. At the same time the residual electric field has to be kept as small as possible. In addition to these requirements, the homogeneity of the B_1 field should be as high as possible to reduce dephasing in the spin ensembles studied. This excludes downscaling of the antennae to the nanometer scale to achieve the highest possible B_1 conversion factors, since this reduces the size of the spin ensemble or results in higher B_1 inhomogeneities in larger samples. To find the optimum stripline structure for spin ensembles we simulated the electric and magnetic fields at the stripline shorts using the software COMSOL 4.3a. The simulation volume was set to a cube with an edge length of 2 cm and perfectly conducting walls. For the silicon sample a cuboid of the dimensions $15 \text{ mm} \times 4 \text{ mm} \times 0.35 \text{ mm}$ positioned in the center of the simulation volume was used. On top of the sample the stripline structure was defined by a perfect electric conductor with infinitly small thickness. The electromagnetic wave was excited by a lumped port with a voltage amplitude of 2 V which corresponds to a microwave power of 40 mW in microwave lines with an impedance of 50 Ω .

Fig. 1 shows slices through the sample at a frequency of 10 GHz for five simulated structures either 2 μ m (panels a, b and c) or 20 nm below the stripline structure (d and e) depicting either B_{1z} (a, b and e) or B_{1x} (c and d). In the following, the structures will be called a to e according to their panel labels. The red squares in Fig. 1a and b depict the area where a contact structure such as interdigit fingers would be placed for EDMR experiments with a B_1 inhomogeneity as obtained from the simulation of less than ± 5%. In Fig. 1c the area exactly beneath the short has a similar B_1 inhomogeneity of less than ± 10%. In structure d the short width is reduced from 20 μ m in structure c to 5 μ m. Although fabrication of a contact structure beneath the short is still possible for this reduced width, e.g. using electron beam lithography, this would increase fabrication complexitiy significantly. Therefore, structure

e is intended to be used as microwave delivery and contact structure at the same time. For this, an additional metallization 5 μ m in front of the 5- μ m-wide short is added. The area beneath the short and the gap between stripline structure and the additional contact in Fig. 1e have a higher B_1 inhomogeneity of up to ± 50%.

All B_1 amplitudes obtained from the simulation quoted below have been divided by a factor of two since for magnetic resonance only one of the two circularly polarized fields contributes to the spin manipulation in the rotating wave approximation. The average B_1 amplitude inside the indicated measurement area is 0.02 mT for structure a and 0.01 mT for structure b which results in expected microwave power-to-B₁ conversion factors of 0.1 mT/ \sqrt{W} and 0.05 mT/ \sqrt{W} , respectively, leading to a power requirement of 13 W and 50 W for 50 ns π pulses, typical for standard commercial pulsed X-band resonators. The average B_1 amplitude inside the measurement area underneath the short of structure c is 0.14 mT, corresponding to a conversion factor of 0.7 mT/ \sqrt{W} and a theoretical power requirement of 260 mW for a 50 ns π pulse. By reducing the short width from 20 µm in structures a, b and c to 5 μ m in structure d, the average B_1 field exactly beneath the short can be increased by a factor of four. With the metal contact in front of the short, a similar average B_1 amplitude of 0.58 mT can also be reached in the gap between the short and the contact. The corresponding conversion factor of 2.9 mT/ \sqrt{W} should allow for 50 ns π pulse times with a power of only 15 mW.

As expected, the simultaneous simulation of the electric field (data not shown) shows that it is smallest at the short where the magnetic field exhibits a maximum and the electric field has a node. Therefore, to reduce the influence of electric fields, the same close proximity of the short and the contact structure already deduced from the optimization of the conversion factor is desirable.

3. Broadband EDMR setup

The setup for broadband EDMR using shaped microwave and radiofrequency pulses consists of three parts: The pulse generation for the excitation of ESR transitions which is presented in Section 3.1, the pulse generation for NMR transitions (Section 3.2) and the detection circuit, which measures the electric response of the sample to the magnetic resonance excitation (Section 3.3). An overview of the setup is shown in Fig. 2.

3.1. Microwave pulse generation

There are two slightly different approaches to ESR spectrometers with pulse shaping capabilites in the literature [24–27]. We use the approach of [24] where pulses are generated at an



Fig. 1. Slices through the sample at a frequency of 10 GHz for five simulated structures depicting B_{1z} (panels a, b and e) or B_{1x} (c and d) either 2 μ m (panels a, b and c) or 20 nm below the stripline structure (d and e). A voltage of 2 V corresponding to 40 mW is applied to the coplanar stripline. The red rectangles depict the measurement area of structures a and b. The measurement area for structure c and d is situated beneath the short, whereas the measurement area for structure e is between the short and the additional contact in front of the short. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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