X BAND ELECTRON PARAMAGNETIC RESONANCE SPECTROMETER BASED ON FIELD PROGRAMMABLE GATE ARRAY

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DEDICATION

This thesis is dedicated to myself.

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ABSTRACT

Electron Paramagnetic Resonance (EPR) is a phenomenon based on Zeeman interaction. To study this phenomenon, a spectrometer is needed. Conventional spectrometers are using benchtop Arbitrary Wave Generator (AWG) or microwave synthesizer as microwave source for continuous wave mode and pulsed mode. However, there are few disadvantages with these instruments. Field Programmable Gate Array (FPGA) is another alternative to AWG due to it advantages such as high flexibility, low profile size and low cost. In this work, a X band FPGA based EPR spectrometer and a loop gap resonator were designed, simulated and built to detect EPR signals. The resonator was measured and found to have an unloaded resonance frequency of 8.852 GHz and Q-factor of 646.0 whereas the loaded resonance frequency was 8.668 GHz with a Q-factor of 615.8. This spectrometer was successfully used to detect EPR signal in an external magnetic field from 311.2 to 311.8 mT with a signal-to-noise ratio (SNR) of 18 ± 8. Based on the experimental parameters, the 2,2-diphenyl-1-picrylhydrazyl (DPPH) g-factor from the developed spectrometer was measured to be 1.9945 ± 0.0012. This value is very close to the DPPH standard value 2.003. Using the designed resonator and DPPH sample, the spectrometer performance such as signal purity, SNR and sensitivity was determined. This spectrometer has the potential to be modified to pulsed mode by installing certain components such as pulse amplifier and power attenuator.

ABSTRAK

Resonans Paramagnet Elektron (EPR) ialah satu fenomena berdasarkan saling tindakan Zeeman. Untuk mengkaji fenomena ini, spektrometer diperlukan. Spektrometer konvensional diperbuat daripada penjana gelombang arbitrari (AWG) atau pensintesis gelombang mikro untuk mod gelombang selanjar dan mod denyut. Namun begitu, terdapat beberapa kelemahan dengan alat-alat terebut. Tatasusunan get logik boleh atur cara medan (FPGA) merupakan satu lagi alternatif kepada AWG kerana kelebihannya seperti fleksibiliti tinggi, saiz profil rendah dan kos rendah. Dalam kajian ini, sebuah spektrometer EPR berasaskan FPGA jalur X dan resonator jurang gelung telah direka bentuk, disimulasi dan dibentuk untuk mengesan isyarat EPR. Resonator tersebut telah diukur dan didapati mempunyai frekuensi resonans tanpa muatan adalah 8.852 GHz dan faktor Q sebanyak 646.0 manakala frekuensi resonans dengan muatan sebanyak 8.668 GHz dengan faktor Q sebanyak 615.8. Spektrometer ini telah berjaya digunakan untuk mengesan isyarat EPR di dalam medan magnet luaran dari 311.2 ke 311.8 mT dengan nisbah isyarat-hingar (SNR) 18 ± 8. Berdasarkan parameter eksperimen, faktor *g* 2,2-diphenyl-1-picrylhydrazyl (DPPH) daripada spektrometer yang dihasilkan diukur sebanyak 1.9945 ± 0.0012. Nilai tersebut adalah sangat hanpir dengan nilai piawai DPPH iaitu 2.003. Menggunakan resonator yang dihasilkan dan sampel DPPH, prestasi spektrometer seperti ketulenan isyarat, SNR dan sensitiviti telah ditentukan. Spektrometer ini mempunyai potensi untuk diubah suai mod denyut dengan memasang beberapa komponen yang bersesuaian seperti amplifier denyut dan pengecil kuasa.

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LIST OF ABBREVIATIONS

EPR	-	Electron Paramagnetic Resonance
AWG	-	Arbitrary Wave Generator
FPGA	-	Field Programmable Gate Array
CW	-	Continuous Wave
DPPH	-	2, 2-diphenyl-1-picrylhydrazyl
VNA	-	Vector Network Analyzer
CNC	-	Computer Numerical Control
LNA	-	Low noise amplifier
ADC	-	Aalog to Digital Converter
DAC	-	Digital to Analog Converter
TLS	-	Two level system
AR-filter	-	Autoregressive filter
RF	-	Radio frequency
Spurious-Free Dynamic Range	-	SFDR
SNR	-	Signal to noise ratio

LIST OF SYMBOLS

B_0	-	External Magnetic field
B_1	-	Driven Magnetic field
S	-	Spin quantum number
ΔE	-	Energy different between ground and excited state
h	-	Plank constant
μ_e	-	Bohr Magneton
T_1	-	Spin-lattice relaxation time
T_2	-	Spin-spin relaxation time
$\vec{\omega}_L$	-	Larmor frequency
$\vec{S}$	-	Spin of electron
g	-	g-factor
f_{Rabi}	-	Rabi frequency
I_x	-	Pauli x metric
I_y	-	Pauli y metric
g_c	-	Spin cavity coupling
ω_o	-	Cavity resonance frequency
Γ	-	Purcell rate
δ	-	Field detuning in the cavity
Q	-	Q-factor
$\dot{M}$	-	Net magnetization of spins,
$M_\perp$	-	Magnetization in x-y plane
M_z	-	Magnetization in z-direction
M_0	-	Initial net magnetization
M	-	Spontaneous net magnetization
N_{min}	-	Minimum detected spins
N_{spin}	-	Total number of spins in sample

BW	-	Bandwidth of the resonance peak
E_c	-	Coulomb energy
E_j	-	Josephson energy
μ_0	-	Permeability of free space
ϵ_0	-	Permittivity of free space
f	-	Resonant frequency of electron spins

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CHAPTER 1

INTRODUCTION

As a small introduction to the structure of this study, chapter 1 discusses the background, problems of current studies in EPR, objectives and aims, research range and importances of this study. Chapter 2 discusses the basic of EPR, hardware in EPR spectrometer and phenomenon associated with the hardware. Chapter 3 discusses the steps and precaution used in designing spectrometer, procedure to test the spectrometer. Chapter 4 discusses the simulation and experimental results for resonator, analysis of EPR spectrometer parameters and analysis of EPR signal from sample. Chapter 5 concludes the work that was done.

1.1 Background of Study

Electron Paramagnetic Resonance (EPR) is a phenomenon of spin excitation of free electron. The theory behind this phenomenon is due to Zeeman interaction in free radical. In other words, any molecules or atoms with at least one free electron have EPR phenomenon. Today, the theory and concept are well known and utilized in various field such as food chemistry [2, 3], protein study [4] and matter structural study [5].

Electron spin is an example two level system (TLS), which is considered as a potential qubit in quantum computing. Quantum information in quantum computer are encoded in the electron spin states. By using EPR, the readouts and quantum operation toward electron spin states becomes possible [6]. The discovery of encoding qubits in quantum dot or spin states of electron in semiconductor is an advancement from the the idea of using spin state of an unpaired electron for quantum computing. However, quantum dot has low coherence time compared to spin qubits in atom that in spin-free environment [7] and the coherence control is a challenging task.

To detect EPR signal, a microwave EPR spectrometer is needed. EPR spectrometer can be used to analyze sample molecular structure, energy levels and other properties related or correlated to electron spin. The EPR spectrometer are commercially available but are designed for general spectroscopy purposes and may not function well for specific purposes such as for quantum computation. For special purpose EPR spectrometer like quantum computing, some parameters must be adjustable or fit a specific sample.

Generally, there are two ways to study EPR: the continuous wave and pulsed. Based on the two method, various methods are derived by varying the experimental parameter or the da data analysis method. EPR spectrometers are designed based on the proposed methods [8, 9, 10, 11].

1.2 Problem Statement

For conventional continuous wave (CW) EPR, microwave synthesizer [10, 12, 13, 14] or Vector Network Analyzer (VNA) [15] can be used as a microwave sources. High stability and accuracy CW EPR spectrometer typically use a lock-in amplifier as this component able to greatly improve the sensitivity of spectrometer [10, 14]. However, the application of CW EPR is limited while pulsed EPR is able to analyze other spin properties such as spin-spin relaxation times, spin-lattice relaxation time and Rabi oscillation [11, 16]. For a more advanced pulsed EPR, expensive arbitrary waveform generator (AWG) is typically used [9, 11, 17, 18]. There are also cheaper alternative methods such as using CW generator with a microwave switch [19]. This alternative method greatly limits the spin manipulation and pulse fidelity as only square pulses are generated [17]. The designs proposed by past researchers required additional microwave receiver such as analog to digital converter (ADC), which increases the complexity for interfacing.

Currently, commercial CW and pulsed EPR spectrometer such as Bruker and Jeol are available [20, 21, 22]. For user friendliness, commercial product reduces the preparation and experimental steps for analyze EPR signals. At the same time, the user loses the flexibility to modify spectrometer parameter such as pulse shape as only square pulses are allowed [22].

A new generation of EPR spectrometer has been proposed and is based on AWG. Thus, AWG is the current main solution for pulsed EPR. However, this arbitrary wave generation is very costly and space consuming especially at X band frequencies and above. Besides this, additional signal receiver might needed for data analysis increasing the profile size of spectrometer [17] and complexity of interfacing program. Due to the high cost for owning an AWG, Field Programmable Gate Array (FPGA) is considered as a cheaper alternative to generate arbitrary wave whilehaving higher flexibility [23].

Besides this, some FPGA is able to incorporate a microwave receiver to become a transceiver to analyse EPR signal which has higher cost effectiveness than AWG based system that need additional microwave receiver to detect the EPR signal. However, suitability of FPGA for signal generation and detection for EPR is still being investigated [24]. Besides, the minimum specification of a homemade FPGA-based spectrometer that can support EPR experiments is still unknown. To that and this study focuses on designing and analyzing the suitability of a homemade FPGA based EPR spectrometer for CW experiment.

1.3 Objective of Study

There are several objectives for this study, that includes:

1. To design and fabricate resonator for X band EPR experiment.
2. To design a working FPGA based CW EPR spectrometer to detect EPR signal.
3. To determine the performance of designed EPR spectrometer such as EPR signal strength, power output and signal purity.

1.4 Research Scope

First, the resonator will be designed, fabricated and analysed. The fabricated resonator must able to generate sufficiently high and homogenous microwave magnetic field, B_1. The FPGA, Xilinx Kintex-7 KC705 is programmed to generate CW with various frequency from 50 MHz to 100 MHz, directed into the resonator containing DPPH sample after passing through signal conditioning component and heterodyning to convert into X band frequency (frequency range from 8 GHz to 9 GHz). The spectrometer circuit will be designed, developed, tested and analyzed. The FPGA based EPR spectrometer must be able to excite electron spin and detect the EPR signal. DPPH sample is used because of DPPH is the standard material in EPR studies and it contains a single EPR peak [25]. Thus, the difficulty to analyze the signal is reduced. The return signals from the resonator is then measured by FPGA and recorded. The data will be analyzed by using a personal computer to determine the EPR signal and other parameters of the spectrometer. The performance of the spectrometer such as EPR signal strength, power output and signal purity will be analysed to ensure the FPGA based spectrometer designed is suitable to obtain EPR signal. Oscilloscope is another choice for measuring the returning signal, but is more costly. This is because the FPGA readings is directly transfer to personal computer without the need of another instrument.

1.5 Research Significant

EPR is widely applied in many fields such as detection of radical, detection and measuring of radioactivity, food industry, oil and gas industry, quantum computing and etc. Moreover, the trend of developing a quantum computer is inevitable. The use of EPR in detection of electron spin state in spin based quantum computer will most likely increase by time [26]. Typically, most of the EPR spectrometer are commercial systems, which are made for general use, user-friendliness but may not be suitable for specific experiment such as quantum computation [27]. Conversely, FPGA based arbitrary wave generation does not has those disadvantages. Firstly, the FPGA is designed by the user where the designed circuit can generate signals for specific purposes to excite the electron spins. FPGA can be designed as a microwave transceiver decreasing the complexity of spectrometer design. Next, the cost of FPGA is much lower than commercial arbitrary wave generator (AWG) especially in high frequency range such as in GHz range. Furthermore, FPGA has low profile size compared to commercial AWG which is important for several purposes such as to cool down the FPGA to improve Signal to Noise ratio (SNR) [28].

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