Optically Detected Magnetic Resonance; Computational Predictions and Experimental Results

Scott Leland Crossen

A senior thesis submitted to the faculty of
Brigham Young University
in partial fulfillment of the requirements for the degree of

Bachelor of Science

Dr. John S. Colton, Advisor

Department of Physics and Astronomy

Brigham Young University

[Approval Month] [Year]

Copyright © [Year] Scott Leland Crossen

All Rights Reserved

ABSTRACT

Optically Detected Magnetic Resonance; Computational Predictions
and Experimental Results

Scott Leland Crossen
Department of Physics and Astronomy, BYU
Bachelor of Science

[The abstract is a summary of the thesis/dissertation with emphasis on the findings of the study. The abstract must not exceed 350 words in length and fit on one page, single spaced.]

Keywords: [A comma-separated list of descriptive words for search purposes]

Contents

Table of Contents **iii**

List of Figures **1**

1 Introduction **2**
1.1 Qualitative Description 2
1.2 5
1.3 5
1.4 5
1.5 5
1.6 5
1.7 5

2 Computational Model and Theory **6**
2.1 7
2.2 7
2.3 Spin Hamiltonians and Defect-State Contributions 7
2.4 7
2.5 7

3 Experimental Methods **8**
3.1 8
3.2 8
3.3 Experiment Background 8
3.4 8

4 Results **9**
4.1 Computational Predictions 9
4.2 Experimental Results 9
4.3 9
4.4 9

Appendix A Electron Spin Studies of Electron Irradiated SiC 11

Appendix B Optical Studies of Cadmium Telluride 13

Appendix C Electron Spin Coherence of Silicon Vacancies in Proton-Irradiated 4H-SiC 14

List of Figures

1.1 Zeeman effect and resonant conditions in matter 4

1.2 Magnetic field and microwave frequency relationship 4

2.1 Example of spin-hamiltonion fields 6

3.1 SiC energy levels and zero-field splitting 8

4.1 ODMR computational model for SiC 9

4.2 ODMR computational model for CdTe 10

4.3 Experimental ODMR for SiC 10

4.4 Experimental ODMR for CdTe 10

A.1 Electron-irradiated SiC lifetime summary 11

A.2 ODMR/Photoluminescence vs temperature 12

B.1 Photoluminescence of CdTe 13

Chapter 1

Introduction

1.1 Qualitative Description

Optically Detected Magnetic Resonance (ODMR) is a particular form of *Electron Paramagnetic Resonance* (EPR) which is more commonly known as *Electron Spin Resonance* (ESR). The latter two of these terms (EPR and ESR) are synonymous; The former (ODMR) is a particular subset of ESR that utilizes a luminescence measuring technique as a means to collect ESR information. In literature, it is common to see both of these terms followed by the designation "spectroscopy" - as that is what they are: tools to study properties of matter via electromagnetic radiation. Though the extent of their application has grown over the years, EPR and ODMR are most commonly used to study the spin-properties of electrons and electron-holes trapped in metal lattices. They can be used to study free radicals in organic materials and are also important in studying the local environment of lattice defects through a technique using angular-dependent ODMR. One particular use of ODMR is the study of electron-spin coherence via a technique known as *Electron Spin Echo*. This can be useful when studying what properties and conditions lead to superior state coherence for qubit candidate materials in quantum computing.

The intellectual foundation of Electron Spin Resonance is rooted in Quantum Mechanics. Bound electrons in matter have discrete and quantized energy levels that govern what frequencies of light are emitted when transitions between energy levels are made. For electron systems, which are fermions and thus subject to the Pauli exclusion principle, the energy levels are 2nd order degenerate when bound in matter. In Quantum Mechanics we choose to describe this degeneracy in terms of spins: we say an electron is either "spin-up" or "spin-down". Each energy level can have at most two electrons of opposite spins inhabiting it (and thus the degeneracy). The spin terminology is moot however, and is really just an attempt to describe electrons as particles - which may be useful for neophytes attempting to learn the material but for our purposes may only confuse the reader to view reality in this way. Furthermore, "electron spin" is a meaningless term unless the "particle" is in the presence of a magnetic field. In this case the energy levels of the molecule will split according to the "zeeman effect" and the spin-states of the electrons can be observed - most commonly through a photoluminescence technique.

Moreover, In the presence of a magnetic field, populations of free electrons will form a spin-1/2 system between a higher-energy "spin-up" state and a lower-energy "spin-down" state. In matter, different parities of spin-states can be formed between the interactions of different energy levels with different transition selection-rules. For a given magnetic-field strength there will be a set of characteristic microwave frequencies that the electrons emit when transitioning between these quantized states. Likewise, for a given microwave target signal, there will be a variety of magnetic field strengths which are most adept at transitioning bound electrons between states. This unique pairing between both the microwave frequency and magnetic field strength is what ESR Spectroscopy essentially is and what it uses to discover information about materials.

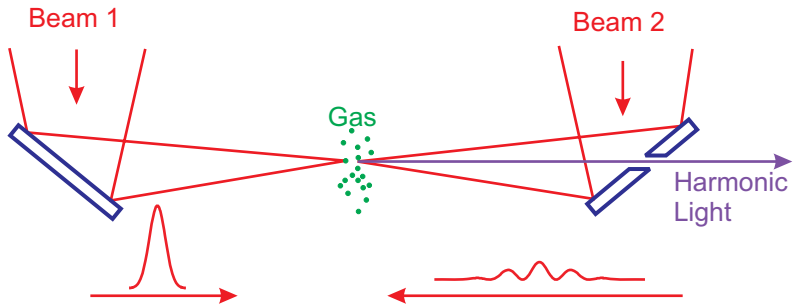

Figure 1.1 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

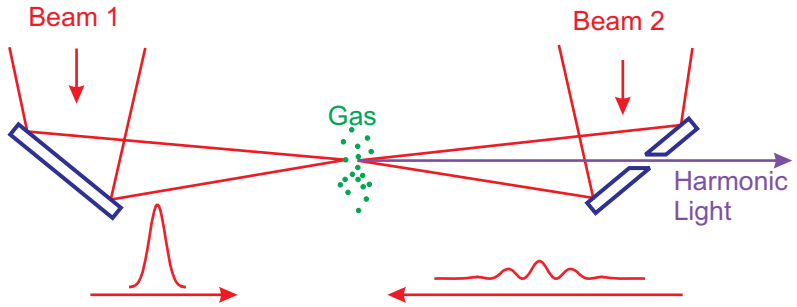

Figure 1.2 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

1.2

1.3

1.4

1.5

1.6

1.7

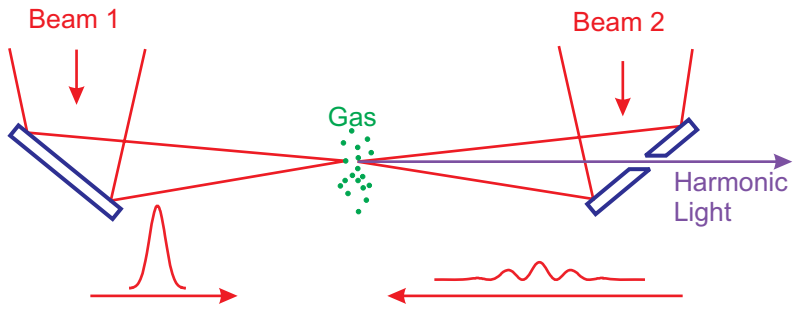

Figure 2.1 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

Chapter 2

Computational Model and Theory

2.1

2.2

2.3 Spin Hamiltonians and Defect-State Contributions

2.4

2.5

Chapter 3

Experimental Methods

3.1

3.2

3.3 Experiment Background

3.4

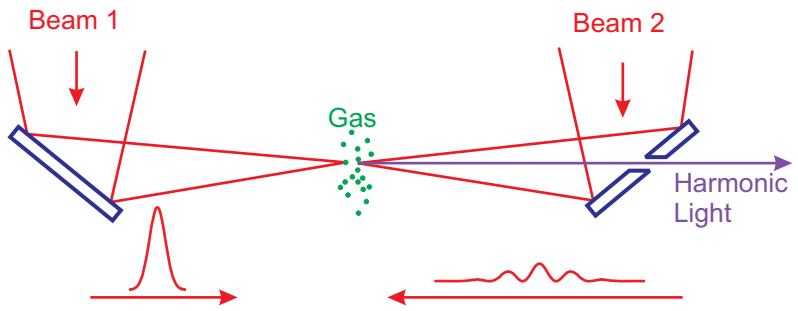

Figure 3.1 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

Chapter 4

Results

4.1 Computational Predictions

4.2 Experimental Results

4.3

4.4

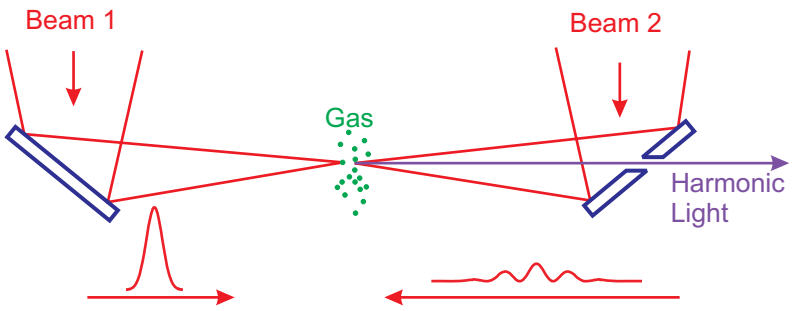

Figure 4.1 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

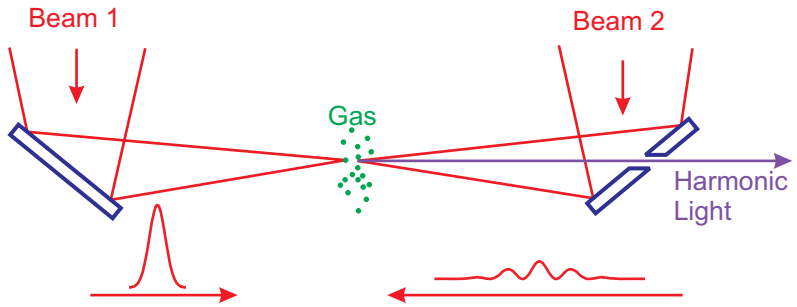

Figure 4.2 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

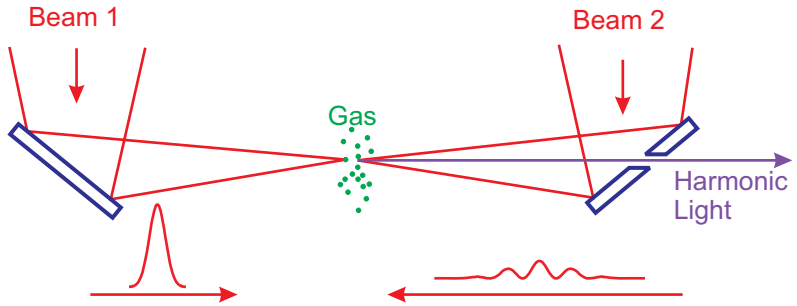

Figure 4.3 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

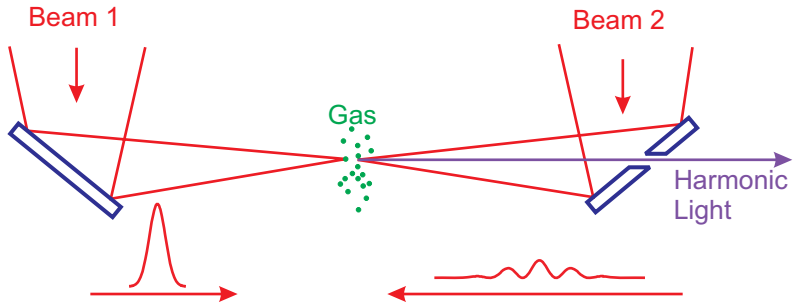

Figure 4.4 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

Appendix A

Electron Spin Studies of Electron Irradiated SiC

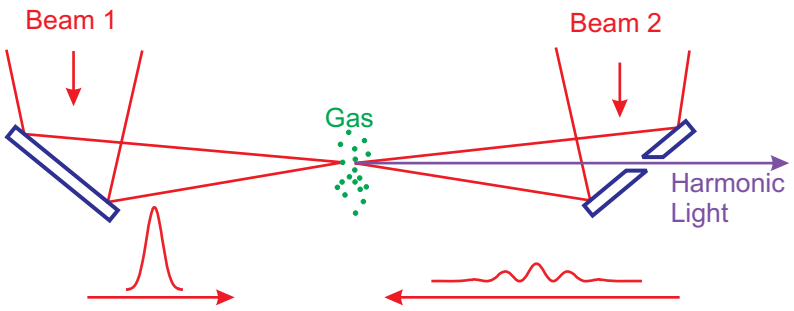

Figure A.1 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

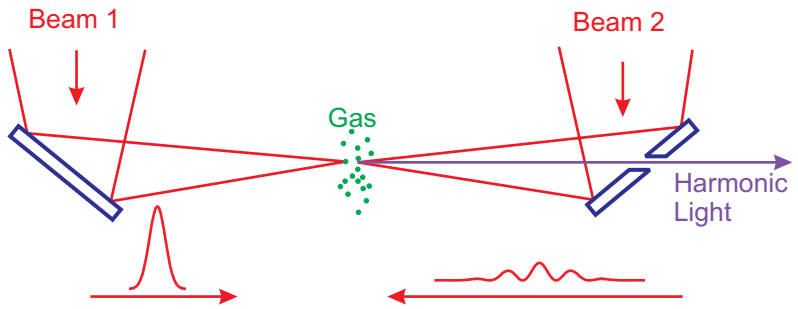

Figure A.2 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

Appendix B

Optical Studies of Cadmium Telluride

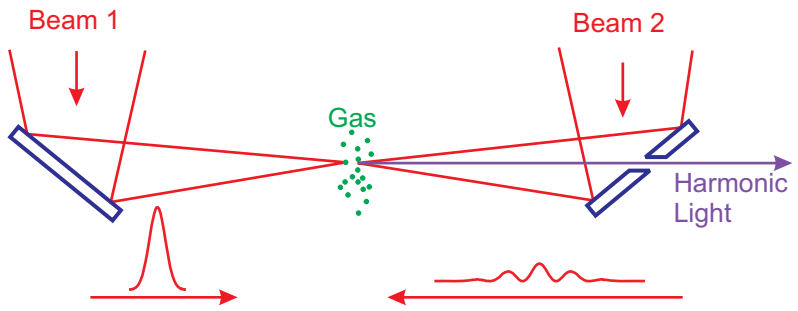

Figure B.1 A mirror with a hole is used to extract high-order harmonics generated in counter-propagating laser beams.

Appendix C

Electron Spin Coherence of Silicon Vacancies in Proton-Irradiated 4H-SiC