MIT Department of Nuclear Science & Engineering

Thesis Prospectus
for the
Bachelor of Science Degree in
Nuclear Science and Engineering

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Development of a Nanoscale Magnetometer Through Utilization of the Nitrogen-Vacancy Defect in Diamonds

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1   INTRODUCTION

The accurate measurement of the magnitude and orientation of small-scale magnetic fields can be beneficial for a variety of scientific endeavors. For example, measuring the magnetic fields of a protein with high spatial resolution can provide information regarding the molecular structure of the protein; similar measurements can be conducted on individual nuclear spins to determine their orientation[1, 2]. The currently used methods of small scale magnetometry, x-ray crystallography, nuclear magnetic resonance and magnetic resonance force microscopy, are either not capable of resolving changes on a nanometer scale, or require cryogenic temperatures in order to operate properly[1]. Thus a new method of magnetometry is required for measurements to be performed in ambient conditions.

A suitable candidate is the Nitrogen-Vacancy (N-V) defect in diamond. This defect occurs when a nitrogen substitutional defect is located next to a vacancy in the lattice structure, which can occur naturally or can be induced through laboratory methods[3]. Of interest to this project is the N-V$^-$ center, in which an additional electron is located within the defect site; by monitoring changes in the spin structure of the N-V$^-$ center, external magnetic fields can be detected.

2   BACKGROUND

2.1   Spin Structure of the Nitrogen–Vacancy Defect

The ground state of this system is a spin-1 triplet. There is a vacuum splitting of the triplet state due to spin-spin interactions such that the energy of the $|0\rangle$ state is lower than that of the $|\pm1\rangle$ states; the splitting is on the order of 3 GHz[2]. This triplet ground state can be excited with 532 nanometer wavelength laser light into an excited triplet state with similar vacuum splitting[1]. The subsequent relaxation process will yield an amount of photons dependent upon the relaxation path. The number of photons depends on the initial polarization of the state: when stimulated, the $|0\rangle$ state will emit more photons than the $|\pm1\rangle$ states. This is due to the finite probability that the $|\pm1\rangle$ states will transition to the $|0\rangle$ state via a metastable singlet state[2], a process known as intersystem crossing (ISC). This transition excites phonons as opposed to photons, so on average the observed number of photons emitted by the $|\pm1\rangle$ states are less than that of the $|0\rangle$ state[3]. Fig.1 gives a visual representation to the spin structure of the N-V$^-$ defect.

It is thus established that the number of photons emitted when optically pumped will be different for the $|0\rangle$ and $|\pm1\rangle$ states for a brief period of time until the system preferably relaxes into the $|0\rangle$ state. The difference in photons emitted during this period is known as the signal photons, and is a measurable quantity[3]. The number of signal photons can provide information about the relative population of $|\pm1\rangle$ to $|0\rangle$ before the system relaxes. Thus, if a perturbation exists that can induce a shift in the relative population of $|\pm1\rangle$ to $|0\rangle$, through analysis of the signal photons one could detect the presence of said perturbation. Furthermore, the drop in photon

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1 It is this unique spin level structure that allows the NV defects to be observed at room temperatures[4]

2 Note: the opposite phenomenon, the $|0\rangle$ transitioning to a $|\pm1\rangle$ state is negligible compared to the probability to radiatively decay.
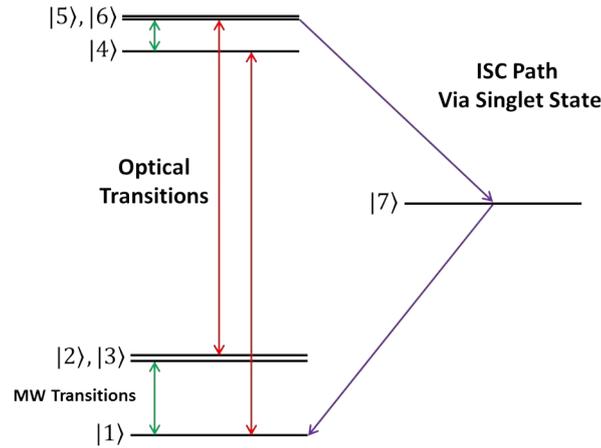
Figure 1: The seven level model in the absence of an external magnetic field, consisting of the ground state and excited state triplets and a metastable singlet. Only spin-conserving radiative transitions and non-radiative transitions to the metastable state are considered.

light intensity may also be observed from optical pumping methods when the frequency is swept through the microwave (MW) range. The drop in intensity signals that the N-V center has been resonantly excited into the $|\pm1\rangle$ state. This method can be used to observe processes that break the degeneracy of the $|\pm1\rangle$ states by monitoring the evolution of the resonant frequencies. An example of this process is shown in Fig.2.

An ongoing field of research is the use of the N-V center to make precision measurements of a small-scale magnetic field; however, with the increased precision comes an expected decrease in simplicity of experimental design. The methods developed in this thesis project aim to accomplish the opposite: a relatively quick and simple method of detecting small-scale magnetic fields at the expense of decreased precision in the measurement. The results of this project can be used to develop a tool for performing fast measurements when complete accuracy is not the primary concern (although nanoscale precision is still obtainable, even with such an "imprecise" device), or an apparatus that can be used in tabletop demonstrations in either laboratory settings or a presentation to a general audience, since the measurement methods will be simple to perform.

2.2 Detection of Magnetic Fields with the N–V Center

It is well known that spins will interact with external magnetic fields such that magnetic moments aligned with the magnetic field lines will occupy a lower energy state than spins anti-aligned to the applied field through what is known as the Zeeman Effect. In particular for the spin-1 triplet ground state of the N-V$^-$ defect in a magnetic field oriented along the N-V spin axis[3], the energy splitting is such that the energy of the $|+1\rangle$ state is shifted

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3 by convention, m_s is taken with respect to the N-V axis
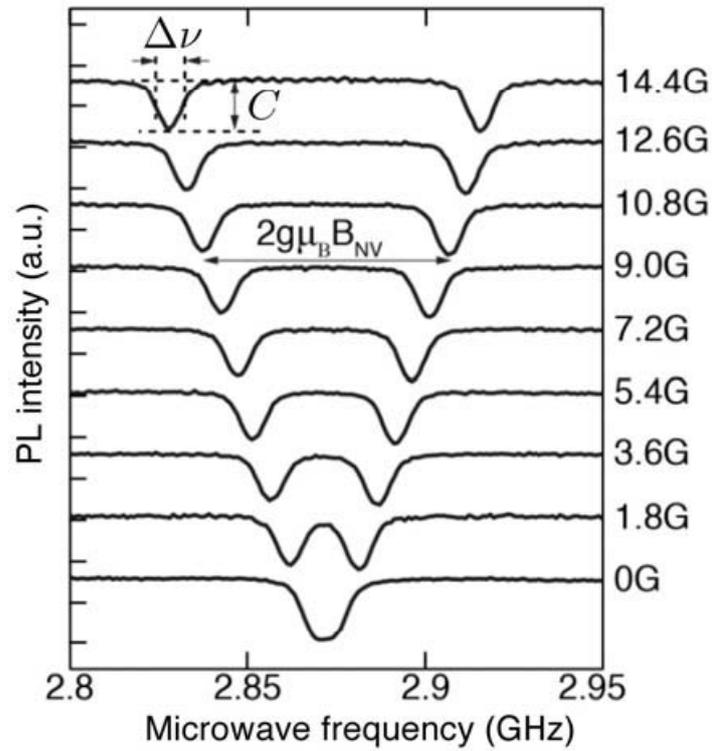
Figure 2: Optically detected electron spin resonance (ESR) spectra recorded for different magnetic field magnitudes applied to a single NV defect in diamond. The ESR transitions are shifted owing to the Zeeman effect, thus providing a quantitative measurement of the magnetic field projection along the NV defect quantization axis. These spectra are recorded by monitoring the NV defect PL intensity while sweeping the frequency of the microwave (MW) field. Spectra for different magnetic fields are shifted vertically for clarity[4].

upward by an amount proportional to the magnitude of the magnetic field, $|-1\rangle$ is shifted downward in energy by the same amount and the $|0\rangle$ state is unaffected. As mentioned previously, this splitting can be observed by performing MW sweeps, as seen in Fig.2.

The diamond lattice has a face-centered cubic structure; correspondingly, there are four possible spatial orientations for the N-V defect[3]. It is expected therefore that an external magnetic field parallel to one N-V center will be at an angle to another N-V center within the sample, necessitating the ability to detect transverse field effects. In transverse fields, the m_s basis with respect to the spin axis is not a good eigenbasis in which to analyze the system, instead, an eigenbasis with respect to the axis of the magnetic field would serve better[3]. Eigenstates in this new basis can be expressed as a superposition of the previous m_s states; consequently there will be a nonzero overlap between the $|0\rangle$ in the new basis and the $|m_s = \pm 1\rangle$ of the old basis. Through this effect, the contrast in photons emitted by the $|0\rangle$ and the $|\pm 1\rangle$ states is reduced; however the net intensity of the photon light is also reduced[4] (see Fig.4). It may therefore be possible to detect the presence of transverse fields by monitoring a change in the intensity of emitted light.

It has been stated that the Nitrogen-Vacancy defect is capable of resolving magnetic fields with nanometer precision at ambient temperatures[1–5]. Indeed, with an optimized pulse sequence, the DC magnetic field sensitivity for a single N-V center can be as low as 40 nT $Hz^{-1/2}$. The AC field sensitivity is even finer due to an increased spin coherence time. Lastly, for ensembles of N-V centers, as will be used in this project, the sensitivity improved by the factor $\frac{1}{\sqrt{N}}$ for N amount of N-V defects in the ensemble[4].

3 OBJECTIVES

This thesis project will aim to develop a simple N-V magnetometer that can be used to detect the presence of small-scale magnetic fields. To accomplish this, it is necessary to create a detection system that can monitor the Zeeman splitting of the ground state energy levels. As discussed in the previous section, the contrast is reduced for transverse magnetic fields, but the intensity of the emitted light is reduced as well. Therefore, a reliable method of detecting the presence of transverse magnetic fields must be developed as well. It should be noted that this project does not aim to determine the magnitude of the external magnetic field, only detect the presence of an external field, simplifying the analysis.

The first step is to understand the current methods of using the N-V center for all-optical magnetometry through a review of literature in this field. The next step is to develop analytically the eigenstates of the ground state manifold and the excited manifold in the presence of a magnetic field. From the expressions of the eigenstates, it is then necessary to calculate the expected photon emission rate. This sequence of steps must be then repeated to account for an ensemble of N-V centers.

After these initial steps, the project will then proceed into optimizing the performance of the N-V magnetometer. In this stage of the project, the first step is to determine the optimal orientation of the external magnetic field that will maximize the contrast in observed photon emission. Once an optimal orientation is determined, the sensitivity of the N-V magnetometer must be established. Thus, the next step is to calculate the minimum magni-
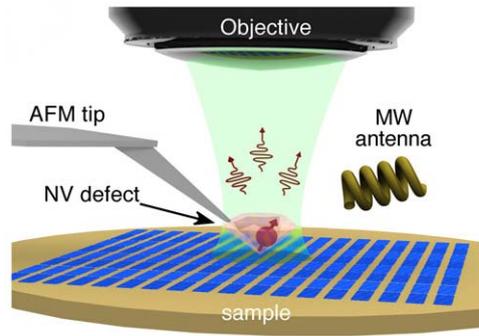
Figure 3: Principle of scanning-NV magnetometry which combines an atomic force microscope (AFM) and a confocal microscope. The AFM tip is functionalized with a single NV defect and a MW antenna is used to perform optical detection of the NV defect ESR transition[4].

tude of the external magnetic field such that the observed contrast is above the threshold contrast value, below which a signal is undetectable. This step concludes the preliminary theoretical analysis. With time permitting, experimental tests are to be conducted regarding the validity of the previous theoretical analysis.

4   METHODOLOGY

The preliminary theoretical analysis is to be conducted as follows: First, to calculate the energy eigenstates of the ground state triplet and excited state triplet through the diagonalization of the governing Hamiltonian. Perturbative techniques are anticipated in the weak field regime; however it may be possible to develop an exact solution. The transition rates must then be calculated such that predictions can be made regarding the observed PL intensity as a function of the applied magnetic field. The field-free transition rates are known from experimentation; it is then straightforward to calculate the effect of magnetic fields on the transition rates through overlapping the vacuum eigenstates with the eigenstates of the N-V system in the presence of a magnetic field. To extend this analysis to ensembles of N-V centers, as will be used in this project, the above steps must be repeated, taking into account the different possible orientations of the N-V center within the diamond lattice.

A common design for an N-V magnetometer is a probe with a diamond tip containing an ensemble of N-V defects that can then be placed over the object of interest. A laser is used for optically pumping the N-V centers; an microwave (MW) spectrum can be used to investigate the spin structure of the N-V centers, as can be seen in Fig.2. Finally, a photon detector is used to register the photon light emitted from the N-V. This photon light can be analyzed to determine information regarding local magnetic fields. A typical setup is shown in Fig.3.

This project will use the all-optical method of magnetic field detection. This technique does not require MW driving and instead monitors the change in PL contrast due to the mixing of the ground level spin states caused by the presence of an external transverse field. This effect can be seen in Fig.4. As stated, N-V magnetometers have been constructed in the past, so there exists an established design that can serve as a strong starting point for this
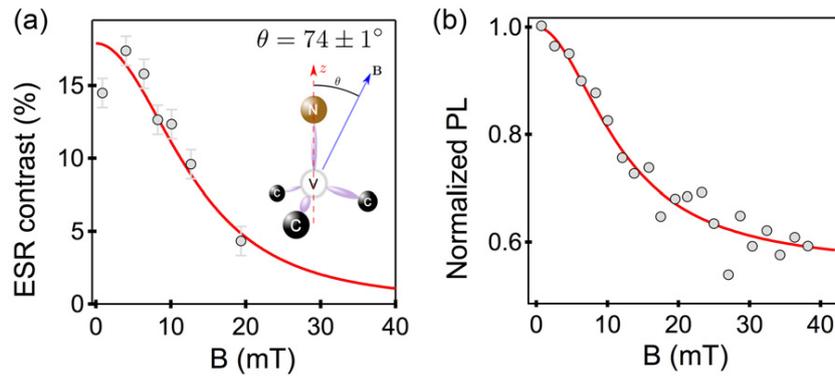
Source: J-P Tetienne et al. New J. Phys. 14 (2012) 103033.
doi:10.1088/1367-2630/14/10/103033. License CC BY-NC-SA.

Figure 4: (a) ESR contrast and (b) normalized PL intensity as a function of magnetic field amplitude applied with an angle $\theta = 74°$ with respect to the NV defect axis[4].

project. Furthermore, Ref.[5] demonstrates an all-optical method of magnetic field detection for a single N-V center; this project aims to expand the all-optical method to an ensemble of N-V centers.

5 SCHEDULE

Present - Jan:	Literature Review
Jan - Feb:	Perform Analytical Analysis of the N-V defect in the Presence of a Magnetic Field
Feb - April:	Experimental Testing and/or Expanded Theoretical Analysis
April - Thesis Due Date:	Write Thesis

REFERENCES

[1] Miller, Johanna. "Diamond Defects Enable Nanoscale Nuclear Magnetic Resonance". *Physics Today* 66: 12-14. 2013.

[2] Childress, Lilian *et al*. "Atom-like Crystal Defects: From Quantum Computers to Biological Sensors". *Physics Today* 67: 38-43. 2014.

[3] Neuman, Philipp, "Towards a Room Temperature Solid State Quantum Processor - The Nitrogen-Vacancy Center in Diamond". *University of Stuttgart, Institute of Physics*. 2011.

[4] Rondin, L, *et al*, "Magnetometry With Nitrogen-Vacancy Defects in Diamond". *Reports on Progress in Physics* 77. 2014.

[5] Tetienne, J-P, *et al*. "Magnetic-Field-Dependent Photodynamics of Single NV Defects in Diamond: An Application to Qualitative All-Optical Magnetic Imaging". *New Journal of Physics* 14. 2012.

22.THT Undergraduate Thesis Tutorial
Fall 2015