Optically Detected Electron Spin Resonance (ODESR): Temperature and Magnetic Field Sensing
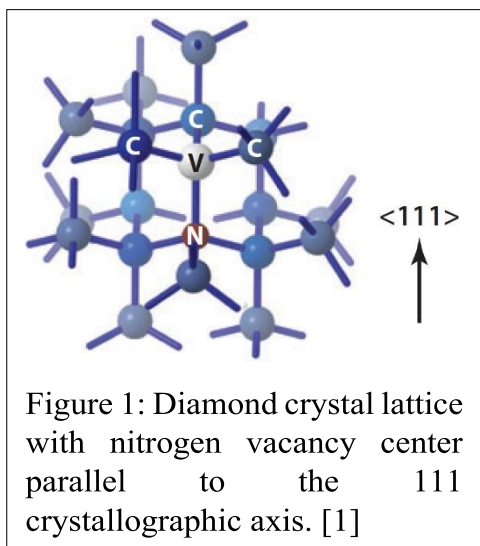
1   Introduction

In this experiment, optically detected electron spin resonance (ODESR), will be used to detect temperature changes in a diamond sample from laser excited fluorescence measurements. From these measurements the temperature dependence of the zero-field splitting (ZFS) D parameter in the spin Hamiltonian will be determined. The ODESR spectrum will also be used to measure magnetic fields, applied with an electromagnet, and the coupling coefficient for magnetic fields will be calculated. With measurements of the magnetic field in both directions, the electric field due to crystal strain in the diamond will be estimated.

2   Theory

Diamond is a crystalline solid composed of sp^3-hybridized carbon. Within the crystal lattice, defects or color centers are either naturally occurring or can be introduced artificially. One such color center, the nitrogen vacancy (NV) center, is the most widely characterized. The yellow coloration of natural diamonds, undesirable in jewelry, comes from nitrogen impurities, however, nitrogen can be intentionally doped into synthetically grown diamonds during high pressure high temperature (HPHT) or chemical vapor deposition (CVD) driven crystal growth. Nitrogen ions can also be doped into an existing crystal via ion implantation, a common method for doping silicon to produce semiconductors.

Vacancies can be introduced into the diamond lattice to form NV centers, usually by electron irradiation to dislodge carbon atoms or as a biproduct of ion implantation. With both types of defect present (nitrogen doping + carbon vacancies), the diamond can be annealed (600-800°C) to cause carbon atoms to hop into vacancies, which in turn causes vacancies to migrate throughout the diamond, usually arriving at the surface, where they are effectively removed from the crystal. When nitrogen defects are present, the unpaired electrons that cannot form covalent bonds to the lattice have significantly higher potential energy, and this potential energy can be minimized if the unpaired electrons localize into a neighboring vacancy, creating a more stable configuration for both defects. This configuration remains stable during annealing. The result is shown in Figure 1.

Figure 1: Diamond crystal lattice with nitrogen vacancy center parallel to the 111 crystallographic axis. [1]

Neutral NV centers possess an unpaired electron. An extra electron can be donated by a second N nearby or by the diamond lattice, to yield a more stable, negatively-charged NV center, NV⁻. This center has an optically excited state that absorbs photons with energy in the green part of the optical spectrum from 500 to 560 nm and decays by emitting deep red fluorescence around 690 nm, shown in Figure 2.

Figure 2: Fluorescent emission spectra from NV⁻ center. [1]
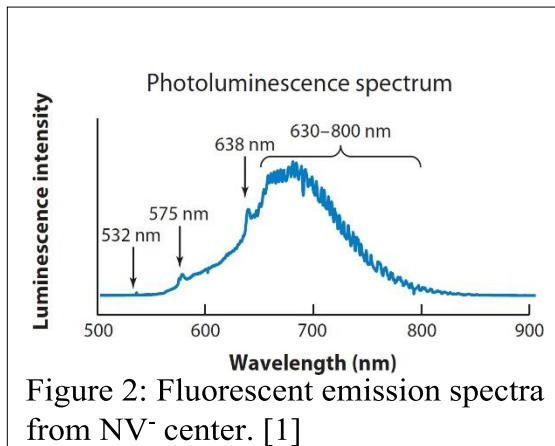
The two unpaired electrons in the ground electronic state of the NV⁻ center are in a triplet spin state (total spin angular momentum=1). The spin projection quantum number can be $m_s = 1, 0,$ or -1 in the absence of an applied magnetic field, the energy difference between the 0 state and the 1 states is $E = \hbar\omega_0$, with $\omega_0 = 2.87$ GHz. This energy is called ZFS. This allows the spin transitions to be excited by oscillating electromagnetic fields in the microwave range.

The optical excitations (ν~560 THz) are spin preserving, meaning they do not alter the spin states.

There is one other important electronic state involved in detecting magnetic resonance from NV⁻ centers; the metastable singlet state labeled as $|s>$ in Figure 3. This state represents an alternative decay pathway from the optically excited state $|e>$ to the ground state $|g>$ that does not emit photon radiation in the visible range. The metastable state has a singlet spin state that is limited to $m_s = 0$ only, and after decaying from this state to the ground state, $|g>$, the NV⁻ center will have $m_s = 0$. As shown in Figure 3, the likelihood of a transition from the excited state, $|e>$, to the metastable state, $|s>$, is strongly affected by the spin state. The result is that if the NV⁻ center has spin $m_s = 0$, there is less than a 2% chance that the electron pair will decay to the metastable state, $|s>$, then to the ground state without emitting light and a 98% chance that it will decay to the ground state, $|g>$, and emit a photon. In contrast, if the NV⁻ center has $m_s = 1$ or -1, there is a 30% chance that it will decay to the metastable state and only a 70% chance of emitting a photon. These dynamics have two important implications for observing ODESR.

Optical Pumping of the $m_S = 0$ State: At room temperature, and in thermal equilibrium, the spin state of a population of NV⁻ centers will be found in a mixture of $m_s = 0, 1$ and -1 states. Because the spin state $m_s = 1$ or -1 increases the likelihood of transitioning to the metastable state, and the metastable state results in a spin $m_s = 0$ state, by repetitively exciting the optical transition (i.e. with a green laser), any NV⁻ centers that were in spin $m_s = 1$ or -1 will end up in the spin $m_s = 0$ state. Any NV⁻ center in the spin $m_s = 0$ has a 98% chance of fluorescent decay (retaining its $m_s = 0$ state, excitation and fluorescent decay are spin preserving transitions), and the 2% chance that it goes to the metastable state both result in the $m_s = 0$ state. NV⁻ centers that originally are in the spin state $m_s = 1$ or -1 have a 70% chance of fluorescent decay (spin preserving), but a 30% chance of transitioning to the metastable state and being converted to the spin $m_s = 0$ state, so on average after a few rounds of excitation, it is likely that NV⁻ centers originally in the spin $m_s = 1$ or -1 will be converted to $m_s = 0$. This process is called optical pumping.
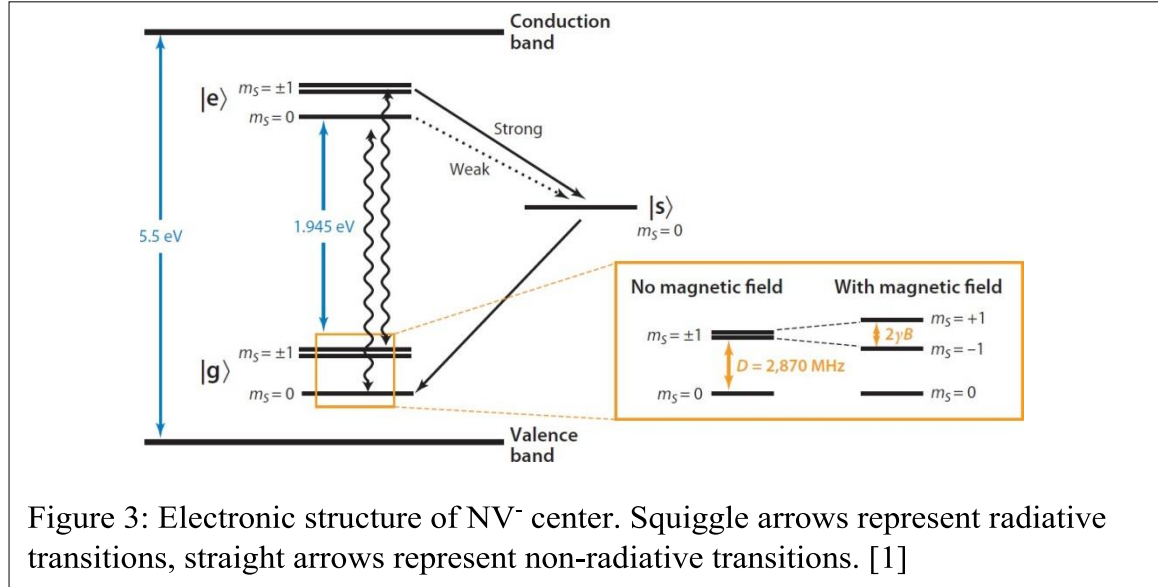
Figure 3: Electronic structure of NV⁻ center. Squiggle arrows represent radiative transitions, straight arrows represent non-radiative transitions. [1]

Pumping means that the spins are initialized into the $m_s = 0$ state, preparing the NV⁻ centers for measurement of microwave induced spin transitions. For comparison, in NMR experiments, a very strong superconducting magnet is used to polarize the nuclear spins; however, only a small fraction of spins (10^{-4}) align with the magnetic field and this small faction of the total spins are then manipulated to provide NMR and MRI measurements. In NV⁻ diamond, we are able to polarize close to 100% of spins via optical pumping.

ODESR and Microwave Induced Spin Transitions: With all NV⁻ spins pumped into the $m_s = 0$ state and the $m_s = 0$ state possessing 98% quantum efficiency for fluorescence output, the fluorescence output is maximized. By applying microwaves at the resonant frequency for the spin $m_s = 0$ to $m_s = 1$ or -1 transition, the NV⁻ center will emit less light as up to 30% of the optical excitations will result in non-radiative decay through the metastable state. By sweeping the microwave frequency, we observe negative peaks (fluorescence drops) in the fluorescent signal when the microwave frequency hits resonance, allowing us to observe the electron spin resonance via fluorescence intensity (depletion).

Energy Levels of the NV⁻ Center Spin States: The energy levels of the spin states define the frequency of microwaves that will activate the transitions of the spin state from $m_s = 0$ to $m_s = 1$ or -1. These energy levels are defined by the spin-Hamiltonian: [1]

$$\frac{H_{spin}}{\hbar} = \underbrace{D\left(S_z^2 - \frac{2}{3}\right)}_{\text{ZFS}} + \underbrace{\gamma\vec{B}\cdot\vec{S}}_{\text{Magnetic}} + \underbrace{\epsilon_z E_z\left(S_z^2 - \frac{2}{3}\right) + \epsilon_{xy}\{E_x(S_xS_y+S_yS_x) + E_y(S_x^2 + S_y^2)\}}_{\text{Electric}} \quad (1)$$

where $D = 2.87$ GHz is the scalar zero field splitting (ZFS) parameter, $\vec{B} = B_x\hat{x} + B_y\hat{y}+B_z\hat{z}$ is the magnetic field vector, $\vec{S} = S_x\hat{x} + S_y\hat{y}+S_z\hat{z}$ is the spin vector, $\vec{E} = E_x\hat{x} + E_y\hat{y}+E_z\hat{z}$ is the electric field vector, and ϵ_{xy} and ϵ_z are coupling constants. The NV⁻ center's main axis is taken to be in the $\hat{z}$ direction (Figure 1). From the Hamiltonian, we can calculate the energy of 3 spin states and the energy difference between them, which determines the resonance frequency of the microwaves required to cause spin state transitions from $E = h\nu$. In weak magnetic and electric fields, the ZFS

3

term dominates and the energy contribution of the spin hamiltonian (H_{spin}) to the total Hamiltonian (H) for each spin state becomes:

$$m_s = -1 \quad \vec{S} = S_z \hat{z} = -\hbar \hat{z} \qquad \frac{H_{spin}}{\hbar} = D\left(S_z^2 - \frac{2}{3}\right) = 2.87 * \frac{1}{3} = 0.957\ GHz$$

$$m_s = 0 \quad \vec{S} = S_z \hat{z} = 0\hat{z} \qquad \frac{H_{spin}}{\hbar} = D\left(S_z^2 - \frac{2}{3}\right) = 2.87 * \left(-\frac{2}{3}\right) = -1.91\ GHz$$

$$m_s = +1 \quad \vec{S} = S_z \hat{z} = +\hbar \hat{z} \qquad \frac{H_{spin}}{\hbar} = D\left(S_z^2 - \frac{2}{3}\right) = 2.87 * \frac{1}{3} = 0.957\ GHz$$

The allowed transitions are governed by selection rules and only $\Delta m_s = \pm 1$ are allowed, resulting in the energy difference for allowed transitions from $m_s = 0$ to $m_s = 1$ or $m_s = 0$ to $m_s = -1$ as $\Delta E = 2.87$ GHz* $\hbar$, where 2.87 GHz is the frequency of microwaves that will result in the correct energy for resonance, driving transitions from the $m_s = 0$ state to either $m_s = 1$ or -1, in the absence of electric and magnetic fields.

3 Apparatus

Figure 4: Diagram of experimental setup
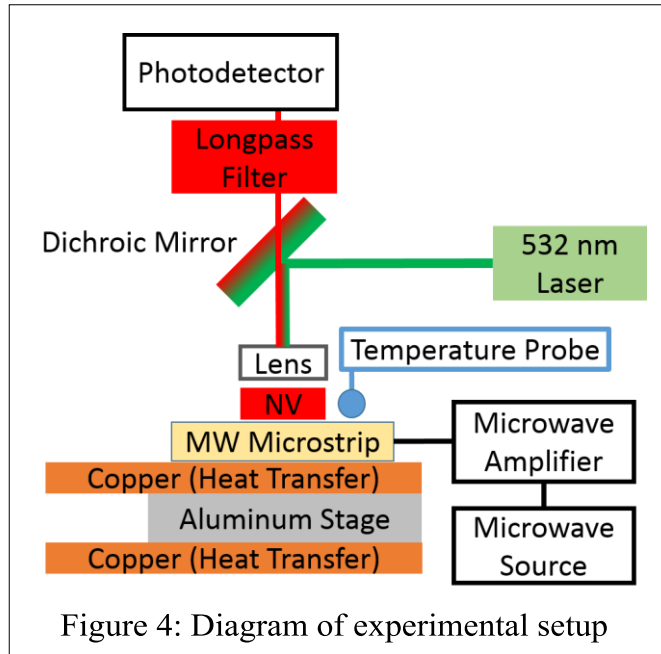
In order to collect the ODESR spectrum, we utilize a standard fluorescence microscopy setup shown in Figure 4 consisting of a 532 nm laser for the excitation source, a dichroic mirror, a focusing objective, a long-pass filter and a photodetector. The dichroic (two-color) mirror reflects light with wave- lengths below 605 nm and transmits light with longer wavelengths. This allows the mirror to reflect the laser light into the lens and to reflect returning laser light back toward the laser source, while transmitting red fluorescent light through to the photodetector.

The diamond is placed under the focusing objective and on top of a microstrip, which acts as an antenna to transmit an oscillating microwave field into the diamond. This oscillating field couples to the NV⁻ centers spins to stimulate transitions when the resonance conditions are met. This effect is described by the rotating wave approximation. [2] This approximation states that an oscillating magnetic field can drive spin transitions when the energy provided by the oscillating field to the spin approaches the energy level of the spin transition, which is $\hbar\omega_0$, where ω_0 is the frequency of the microwave signal when on resonance.

4 Procedure

Initial Measurement: Turn on the laser (black box labeled: 532 nm 180 mW LASER), photodetector (small black GlobTek transformer), microwave amplifier (BK Precisions), oscilloscope (Tektronix 2012B), and function generator (Rigol DG4162, you will have to push hard on the power
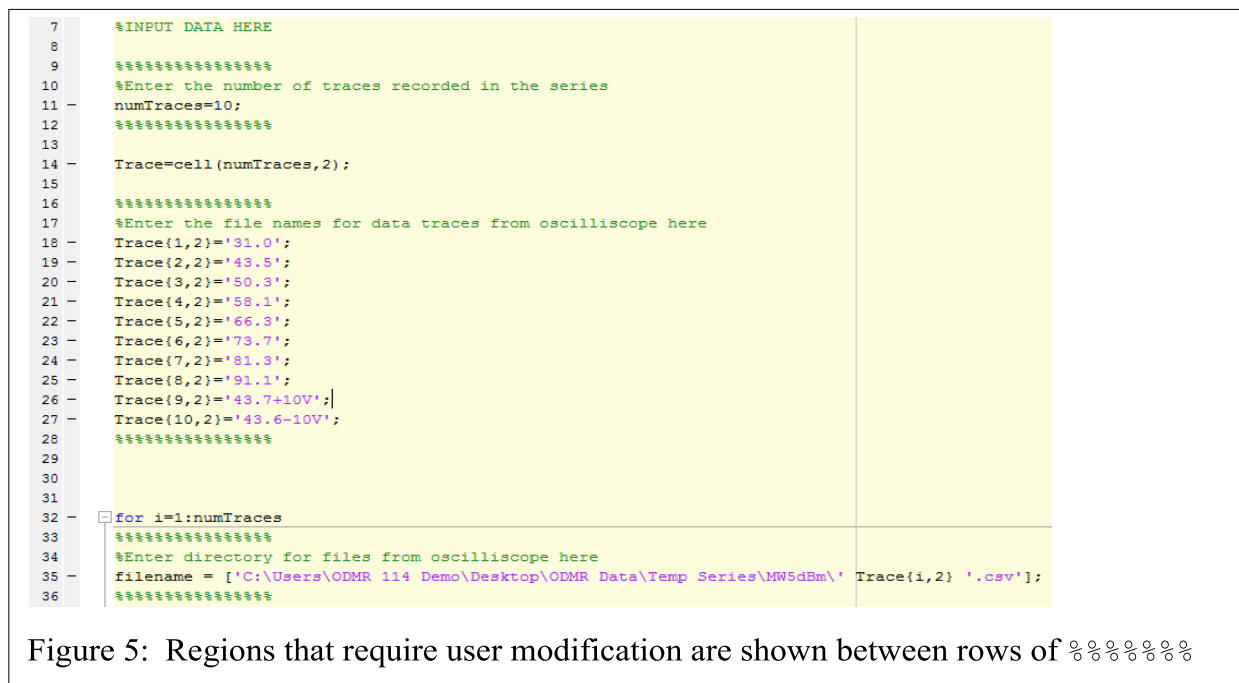
switch). Open the LabView DG4162 program on the computer desktop and run it with Channel 2 OFF (click once the top left white arrow). In a few seconds you should see a signal on the Oscilloscope (yellow trace), that represents the fluorescence from the diamond. Turn on the sample thermometer (Fisher Scientific) and wait a few minutes (at least 5 min) for the temperature to stabilize. Open SynthHD1_0 and click "RF is Off". It should turn red and read "RF is On". The yellow signal on the oscilloscope should develop two inverted peaks (depletion of the fluorescence). Monitor the temperature until it stabilizes anywhere from 23°C to 26°C. Allow the temperature to stabilize until the change is less than 0.1°C every 2 minutes. Position the yellow signal vertically in the middle of the screen. While you are doing this, notice the number of offset divisions in the lower part of the oscilloscope screen in red (should be a number in the -50 to -90 range). Open LabView Tek2012B. Enter the Vertical Offset, make sure the RUN/STOP button is in RUN mode, and start the software. It takes ~15 sec to measure the first spectrum. Collect ~100 averages and record the temperature of the stage every 2 minutes to monitor the stability. If the temperature drift is too high, you can continue the averaging for additional two minute intervals until you have a few minutes of averaging with stable temperature (the minimum acceptable stability is 0.1 °C per 2 min, but stability of 0.1 °C per up to 12 minutes is achievable). Stop the software by pressing RUN (will show STOP for a second). The program will stop a few seconds later. Right-click inside the graph and select Export/Export Data to Excel. An Excel spreadsheet will open. Delete the first row (labels) and Save As CSV (comma delimited), naming your file with the run temperature (i. e. 27.3)

Temperature Series: Turn the hot plate ON and set temperature to 500°C by removing the orange lid and grey weights on top of the orange box. Put the lid and weights back in place. Monitor the temperature on the Fisher thermometer until it reaches 95°C, then turn the hotplate down to 400°C and allow it to stabilize until the temperature change is less than 0.1°C in two minutes. This should take about 20 minutes. After the temperature stabilizes, adjust the vertical position on CH 1 of the oscilloscope (more negative values at higher temperatures) until the yellow waveform is centered and input the vertical offset (divs) in the software. Start the LabView data collection and average for several minutes (hopefully the same # as before) recording the temperature of the stage every two minutes. Export data as before.

Next, remove the lid from the box and adjust the temperature of the hot plate to 350°C. Replace the lid and weights and monitor the temperature until it stabilizes to less than 0.1°C in two minutes. This stabilization should take about 15 minutes. After the temperature has stabilized, re-center the vertical position on the oscilloscope, input vertical offset and collect data. Record the temperature every two minutes. Repeat this process for 300, 250, 200, 150, 100, and 50°C set points on the hotplate.
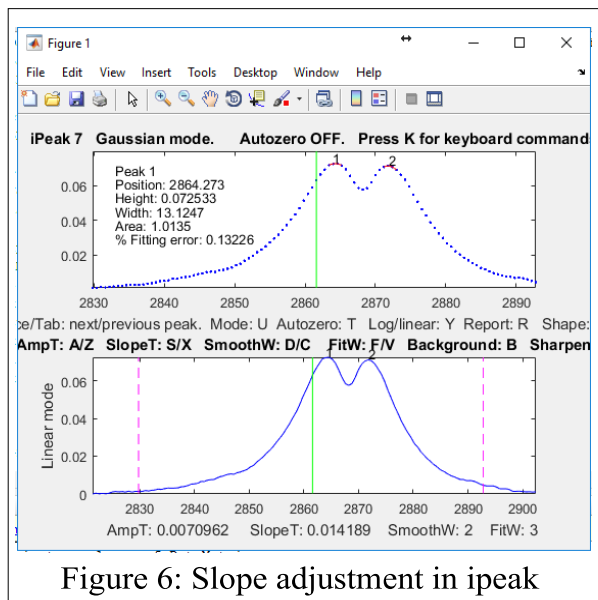
Magnetic Field Measurement: With the hotplate at 50 °C, wait for the temperature to stabilize. Open the DG4162 program. Turn Channel 2 ON, type 9 on the Channel 2 Voltage and run the program. This will apply a constant 9 V to the magnetic coil attached, and will generate a constant magnetic field in the vertical direction. The coil is located above the lens. Adjust the oscilloscope vertical position, input vertical offset and collect data, recording the temperature every 2 min. Name the data file, for example, 9V35.5 (where 35.5 is the temperature). Repeat this for 9.25, 9.5, 9.75, and 10 V. Next collect a series with the magnetic field reversed at -9, -9.25, -9.5, -9.75, and -10 V for a total of 10 magnetic field traces (you need to collect 10 traces in order to use the MATLAB analysis routines discussed below). This will allow us to calculate the gyromagnetic ratio, or γ, of the NV⁻ spin in the magnetic field term of the Hamiltonian.

PLEASE, TURN the INSTRUMENTS OFF when you are done (including the hot plate).

```
 7        %INPUT DATA HERE
 8
 9        %%%%%%%%%%%%%%%%%
10        %Enter the number of traces recorded in the series
11 -      numTraces=10;
12        %%%%%%%%%%%%%%%%
13
14 -      Trace=cell(numTraces,2);
15
16        %%%%%%%%%%%%%%%%%
17        %Enter the file names for data traces from oscilliscope here
18 -      Trace{1,2}='31.0';
19 -      Trace{2,2}='43.5';
20 -      Trace{3,2}='50.3';
21 -      Trace{4,2}='58.1';
22 -      Trace{5,2}='66.3';
23 -      Trace{6,2}='73.7';
24 -      Trace{7,2}='81.3';
25 -      Trace{8,2}='91.1';
26 -      Trace{9,2}='43.7+10V';
27 -      Trace{10,2}='43.6-10V';
28        %%%%%%%%%%%%%%%%
29
30
31
32 -  ⊟ for i=1:numTraces
33        %%%%%%%%%%%%%%%%%
34        %Enter directory for files from oscilliscope here
35 -      filename = ['C:\Users\ODMR 114 Demo\Desktop\ODMR Data\Temp Series\MW5dBm\' Trace{i,2} '.csv'];
36        %%%%%%%%%%%%%%%%
```

Figure 5: Regions that require user modification are shown between rows of %%%%%%%

5   Data Analysis

Plot, Normalize and Average Traces: Open the MATLAB file ProcessTraceTemp.m found in the folder `C:\Users\Lab User\Desktop\114 ODMR Analysis`. Use the "Save as" command to save this file in your data folder. In the analysis script, the sections that require input are surrounded by %%%%%%% shown in Figure 5. Enter the number of temperature traces that you recorded, which should ideally be 8-10. Scroll down to the first row where it says `Enter the file names for data traces from oscilloscope here`. In between the single quotes on each line, enter the file names for each temperature trace and the magnetic field traces. Next, enter the name of the folder where your files are located into the first array element of the filename (line 35 in Fig 5). Press `Run` on the upper menu to execute the script, which should generate 3 figures: The raw traces, the baseline normalized traces, and the ODMR signal at each fixed frequency. Save these figures for your report.

Figure 6: Slope adjustment in ipeak

The script plots the raw traces recorded from the oscilloscope (first figure), normalizes the signal to the baseline with zero microwaves applied (second figure), then takes the values recorded for each microwave frequency step and averages them to output the ODMR signal at that frequency.

Peak Fitting for Temperature Series: To determine the center location of each individual peak, you will use ipeak, a peak analysis module written for MATLAB. Open `ipeak.m` from the `C:\Users\Lab User\Desktop\114 ODMR Analysis` folder and save it in your data folder. Execute the script to enable use of the ipeak function. Load the first trace for analysis using ipeak using the MATLAB command: Type `ipeak(MWFreq,aveODMR{1})` on the command window.

This will use the values stored in the array `MWFreq` as the x axis values and the first averaged ODESR trace for fitting. After running this function, an interac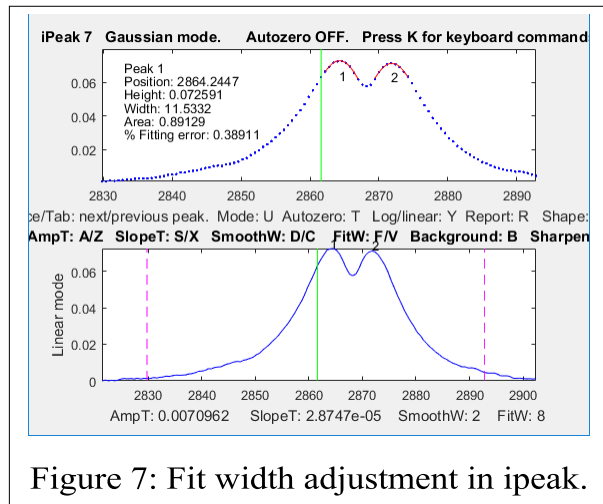tive figure will open. Press 'Shift+G' to toggle the mode from Gaussian to Lorenztian peak mode. Repeatedly press the down arrow key to bring the full curve into view in the top window. Next, press the x key several times to lower the maximum slope for peaks until 1 and 2 appear above each peak. Next, press `f` approximately 5 times to broaden the fitting width of the preliminary peak estimate (pink curve) so that the estimate extends to both sides as shown in Figure 7, without overlapping. To perform multiple peak fitting, press `m` and in the MATLAB command window; a dialog box asking for peak shape will appear. Press `2` and hit enter to select a Lorentzian function as the equation to fit peaks to. For number of trials, enter 100.

Figure 7: Fit width adjustment in ipeak.

A second figure will appear showing the fitting results and the peak information will appear in the MATLAB command window. Verify that the fit is reasonable. Figure 8 gives an example of the expected fit. To record the peak fitting results, copy them into the `TempPeakResults` data structure created by the script with the command: `TempPeakResults{#} =P` where the # is the trace number used for the fitting.
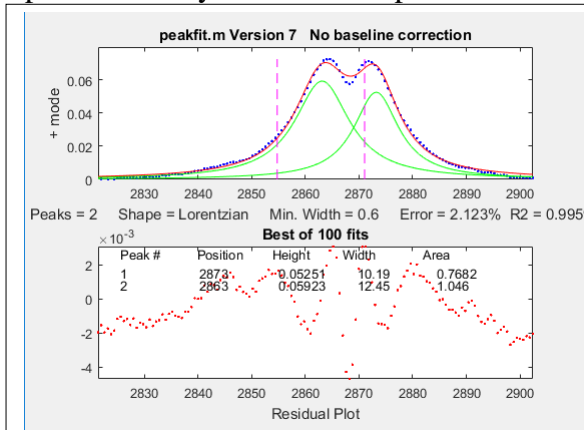
Repeat this analysis for all temperature traces. The command to load each new trace into ipeak is: `ipeak(MWFreq,aveODMR{#})` where # is the trace number. Next, create 2 plots of temperature vs peak center for peaks 1 and 2. To do this, first generate the x axis of temperature values in MATLAB by defining an array of the temperature values recorded while taking the temperature traces. Do not include the traces taken with the magnetic field on. The syntax is:

`Temperatures=[31.0 43.5 50.3 58.1 66.3 73.7 81.3 91.1]`

Figure 8: Fitting results from ipeak.

Next, create the Y axis from the peak centers:

`for i=1:8; Peak1(i)=TempPeakResults{i,1}(1,2); end;` and `for i=1:8; Peak2(i)=TempPeakResults{i,1}(2,2); end;`
Now generate a plot of the data in a new figure using the command:
`figure; plot(Temperatures,Peak1,Temperatures,Peak2)`
Format the figure and identify the peak data in the legend with these commands:

```
legend('Peak1','Peak2')
xlabel('Temperature ^{\circ} C')
ylabel('Microwave Frequency (GHz)')
title('Temperature vs. Microwave Frequency for m\_s=0 to -1 and
m\_s=0 to 1')
```

In the figure's Tools dropdown menu, select Basic Fitting. In the Basic Fitting window, at the top select data as Peak1 and under Plot fits check linear. Click on the arrow at the bottom of the window to display the next window and record the fitting coefficients p1, p2 and the norm of the residuals. Ensure the show equations check box is checked, and save the figure in JPEG or PNG file format.
For the second peak, in the Basic Fitting window, select Peak2 under select data, record the coefficients p1, p2 and the norm of the residuals, ensure that the show equations box is checked and then save the figure again with a different name for your report. The slope of the linear fit, the coefficient p1, gives the measured value for the temperature dependence of the ZFS term in the Hamiltonian, equation 1, with units of GHz/°C. Compare the value of this parameter to the literature value. [3]

Plot, Normalize and Average Magnetic Field Traces: Open the MATLAB file 'ProcessTraceMagField.m' from folder `C:\Users\Lab User\Desktop\114 ODMR Analysis` and save it in your data folder. In the analysis script, the sections that require input are surrounded by `%%%%%%%%%` shown in Figure 5. Enter the number of traces that you recorded, that *has to be* 10 for this program to work. Scroll down to the first row where it says `Enter the file names for data traces from oscilloscope here`. In between the single quotes on each line, enter the file names for each magnetic field trace. Next, enter the name of the folder where your files are located (line 35 in Fig 5). Press `Run` on the upper menu to execute the script, which should generate 4 figures: The raw traces, the baseline normalized traces, and the ODMR signal at each fixed frequency for the negative and positive voltages. Save these figures for your report.

Peak Fitting for Magnetic Field Traces: Load the first magnetic field trace into ipeak using the command: `ipeak(MWFreq,aveODMR{#})` where the # is the trace taken with 9 V applied to the magnetic coil, ideally 1. In the interactive ipeak window, press the down arrow until the full curve is shown in the upper window. Press `x` several times (10-20) until the numbers 1,2,3, and 4 are shown above the 4 peaks. Reduce the smooth width to 1 by pressing `c` once. Extend the preliminary fit width by pressing `f` 8 or 9 times. Press `m` to fit the multiple peaks, followed by entering option 2 in the MATLAB command window to select Lorentzian functions, and enter `100` for the number of trials. After the fit is complete, save the peak results into the data structure MagPeakResults using the command:
`MagPeakResults{#}=P` where the # is the trace number used for fitting. Repeat this process for all of the magnetic field traces.

Analysis of Magnetic Field Traces: From the second term in the Hamiltonian (1), the energy contribution of the magnetic field to a given state depends on the dot product of the spin vector and the magnetic field vector. To calculate the energy of the transition from $m_s = 0$ state to either $m_s = 1$ or -1 it is necessary to know the direction of the spin vector and the magnetic field. For the NV⁻ spin direction, we have to remember that the NV defect is aligned in the same direction as the carbon bonds found in the diamond. Bonds between carbon atoms in diamond have sp^3 hybridization, with 4 possible orientations, each with 109.5° bond angles between them. Similarly, the NV⁻ centers generally form equally in all 4 possible orientations. An applied magnetic field will contribute to the

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energy of each NV⁻ center differently depending on its direction.

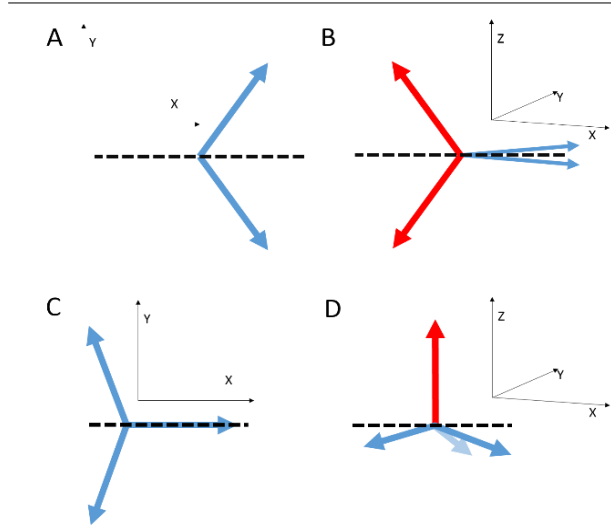In this experiment, we are using a diamond with the crystal oriented with either the [110] or [111] plane facing up. For the [110] diamond, there are two bonds oriented in the x y plane (in the plane of the table top). The other two orientations can be found by taking the line that bisects the 109.5°angle between the first two directions and extending it as a unit vector in the opposite direction, then tilting the unit vector into the positive and negative z direction by 54.75°, to give a 109.5° bond angle, as shown in Figure 9 A, B. With a magnetic field from the coil being applied in the z direction, it should be clear that we end up with 2 unique cases. The two NV⁻ orientations in the x y plane are perpendicular to the magnetic field, which yields a dot product of 0 and should not change the energy of the transitions. The two orientations that have some component in the z direction will have a change in the energy of the transitions, with equal magnitude and opposite directions, resulting in the same magnitude of change in the transition energy. In this experiment, changes in the transition energy appear as shifts in the resonant frequency, which shifts the peaks locations in the ODMR spectra.

Figure 9: A: 2NV⁻ directions in *x-y* plane. B: 4 NV⁻ directions for [110] crystal orientation: 2 in *x-y* plane (blue), 2 rotated opposite ways in the z direction. C: 3 symmetric NV⁻ orientations in the *x-y* plane. D: 4 NV⁻ directions for [111] crystal orientation

The [111] crystal orientation has three fold symmetry in the x y plane as shown in Figure 9 C. The fourth bond orientation is in the z direction, with the other three projecting into the x y plane and into the z direction, as shown in Figure 9 D. With a magnetic field applied along the z direction, there are only two unique cases. One orientation parallel to the z axis, and three directions that form degenerate projections onto the z axis, making 109.5°angles with the z axis, resulting in the spin projection onto the z axis being scaled by cos(109.5°).

To get started on the analysis, open the file `AnalyzeMagFieldSeries.m` from folder C: Users\ Lab User\ Desktop\ 114 ODMR Analysis. Use the `Save as` command to save this file in your group's folder. This file will plot the absolute peak separations from the data collected in the `MagPeakResults` structure for positive currents and negative currents, as well as the peak separations relative to the peak separations from the lowest magnitude current trace (i.e. peak separations from traces taken with 9V or -9V on the function generator).

The voltage setting on the function generator can be converted to the current flowing through the coil by knowing that the equivalent circuit for the coil has a resistance of 64.5 Ohms. For a solenoid, the magnetic field along by the z axis can be found by

$$B_z = \frac{\mu_0 I n}{2} \frac{r^2}{(z^2 + r^2)^{3/2}}$$

To interpret the magnetic field measurement, it is necessary to include the direction of the NV⁻

centers in order to determine strength of the applied magnetic field, B. B is a vector quantity, $\vec{B} = B_x\hat{x} + B_y\hat{y} + B_z\hat{z}$. When B is applied along the z direction, we write $\vec{B} = B_z\hat{z}$. This makes the dot product in the magnetic field term of equation (1): $\vec{B} \cdot \vec{S} = B_z S_z$. The spin vector, $\vec{S}$, is a vector of length $\hbar\sqrt{s(s+1)}$, where s=1 is the spin. Its z-projection can be $S_z = -\hbar, 0, \hbar$. The orientation is important because the magnetic field term is $\gamma\vec{B} \cdot \vec{S}$ and the magnetic field is in the Z direction, so the z projection must be scaled according to the angle between the NV$^-$ direction in question and the z axis. For example the two NV$^-$ orientations in the [110] crystal orientation with a z component are scaled by $sin(109.5°/2)$.

Report Questions and Calculations:

1. Compare the values of the coefficient of the zero field splitting obtained from your temperature series measurements (i.e. the slope from the linear fit) from both peaks to the literature value in reference [3]. Explain in your own words what this coefficient represents and give its proper units.

2. For the temperature series, calculate the peak separation in MHz (p2- p1) and calculate the average and standard deviation for the temperature series. What is the energy difference between the two states represented by these peaks? (value and units) What term in the Hamiltonian contributes to this energy?

3. Using equation 2, the calculated currents from V=IR, the literature value for the NV$^-$ gyromagnetic ratio [1] and your peak measurements from the magnetic field series to determine a coil characteristic constant (Q) for the coil that includes the number of turns, the distance from the coil to the diamond, and the coil geometry by solving $\Delta B = Q\Delta I$, where Q includes μ_0, n, r and z. μ_0 is 12.56637 G mm/A when converted to the relevant units.

4. Fit the slope of the line for the peak locations from the magnetic field data vs. the current for the outermost peaks (p4-p1) and innermost peaks (p3-p2) for the positive and negative magnetic field traces. Use the literature value [1] for the gyromagnetic ratio of the NV$^-$ center to calculate B, the magnetic field at the diamond. Comparing the relative shift of the two pairs of peaks, is the data most consistent with the diamond surface having a [111] or [110] crystal orientation? Why?

5. Notice that the positive and negative currents do not result in identical peak shifts. Calculate the energy difference between the outer peaks for each pair of positive and negative currents (i.e. traces taken at 9 and -9 V, 9.25 V and -9.25 V, etc.) using the literature value for the gyromagnetic ratio [1] and D [3] parameter. For the outer peaks of the highest current pair (10 V, -10 V), calculate magnetic field term of the hamiltonian. Use this calculated value and the energy difference calculated from the ODMR spectra to solve for the contribution of the electric field parameter to the Hamiltonian. Using this value and the literature value of z [1], calculate the electric field present in the diamond along the Z axis, E_z.

References

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