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An Overview of NV Centers

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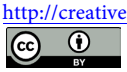

Abstract

This paper is a literature review on the operating theory of NV centers and its applications. Extensive material online had been reviewed to provide a comprehensive explanation of NV centers in this literature review.

Keywords

NV Centers, Functions, and Applications

1. Introduction

Quantum sensors are the basis of many important modern technologies, such as the magnetic resonance imaging (MRI) and the detection of greenhouse gasses in the earth's atmosphere. Because they measure physical quantities—heat, sound, light, pressure, and electromagnetic fields, among others—using atomic scale systems, quantum sensors have incredible precision and accuracy, with their abilities hovering high above those of classical sensors. This paper is a literature review on the operating theory of one type of quantum sensor, the NV center, and its applications.

2. NV Centers and How They Work

2.1. NV Centers and Its Structure

One of the many quantum sensors widely used by scientists today is Nitrogen-Vacancy Centers, known as the NV centers. NV centers are defects where one carbon atom lying next to a vacancy (a "missing atom") is replaced by one nitrogen atom in a diamond crystal or thin film, resulting in a mobile electron and a nearby vacancy [1]. This is an NV center (see also **Figure 1**). They can be natural, or created artificially and controllably by a variety of methods. One such method is irradiation [2] [3] providing a nitrogen atom some energy (at high temperatures) so it can break the covalent bonds between carbon atoms and re-

place a carbon atom. Since this NV center gains no electrons from its external environment (*i.e.*, the lattice structure surrounding it) and only has 1 unpaired electron, it is called an NV^0 [1] [3].

However, in quantum sensing, NV^{1-}, where the defect site gains an electron and has 2 unpaired electrons at the vacancy, is of particular interest. Having a quantum state with two electrons yields a total spin $S = 1$, which then splits into three quantum sublevels indexed by the quantum number $m = -1, 0, +1$. The acquired electron comes from the isolated Nitrogen atom in the lattice structure such that the net charge of the overall system remains the same [4].

2.2. Energy Levels in NV Centers

NV centers are *artificial atoms*, whose energy levels are discrete, like those of actual atoms. The discovery of the energy level quantization in atoms was one of the seminal discoveries of the first quantum revolution in the early 1900's. Electrons occupy a region outside the atom's nucleus at certain special locations called "orbitals" (**Figure 2**). Each orbit corresponds to a certain amount of

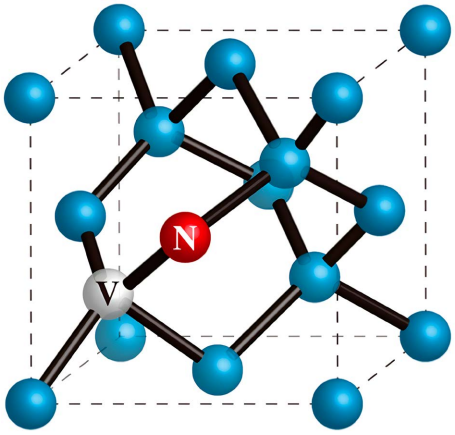

Figure 1. Diagram of NV center.

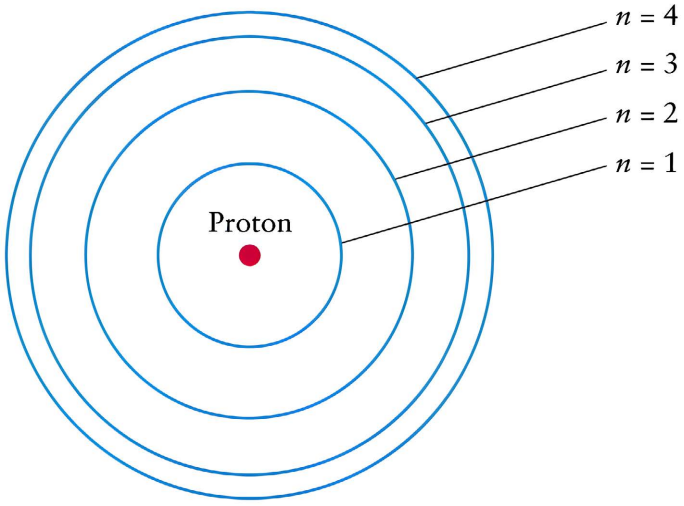

Figure 2. Bohr model of hydrogen.

energy called the energy level, which means energy levels are discrete. This is the model that was originally developed by Danish physicist Niels Bohr [5]. The different energy levels are enumerated with an integer label n, known as the *principal quantum number*. In the case of hydrogen, according to Bohr's model, if its electron is at the $n = 1$ energy level, the atom is at its ground state. If the electron has energy levels greater than $n = 1$, the atom is in an excited state.

We can identify two main sets of quantum states in an NV center: ^{3}A, triplet ground state, and ^{3}E, triplet excited state. Each triplet state has 3 different spin states: $|0\rangle$, $|-1\rangle$, $|+1\rangle$. Initially, these 3 spin states are "degenerate"—they have the same energy level. However, because of the intrinsic magnetic environment provided by the lattice structure, the $|0\rangle$ state splits with $|\pm1\rangle$ states. This is called the zero-field splitting (ZFS) and it is due to spin-spin interactions which are influenced by the lattice [6] [7]. These formerly degenerate levels now have different energies. In addition to these two main sets of states, there is an intermediate singlet state between the ground and excited energy states [8]. The latter plays an important role in the radiative processes that connect the ^{3}A and ^{3}E states. There is no external magnetic field applied at this point. An illustration of the energy levels is shown in **Figure 3**.

To excite the spins *coherently*, namely so the NV center can be in a quantum superposition of $|0\rangle$ or $|\pm1\rangle$, an electromagnetic wave is used to excite the NV center. In this case, a microwave pulse is required [8] because the energy splitting between the levels is in the range of electromagnetic radiation with frequency in the GHz frequency range. For instance, to reach the ^{3}A $|\pm1\rangle$ states from ^{3}A $|0\rangle$ state (without an external magnetic field applied), a microwave pulse at a frequency of 2.87 GHz needs to be directed at the NV center (**Figure 3**) [9].

2.3. Zeeman Effect

If there is a magnetic field applied to this system, the Zeeman effect would take

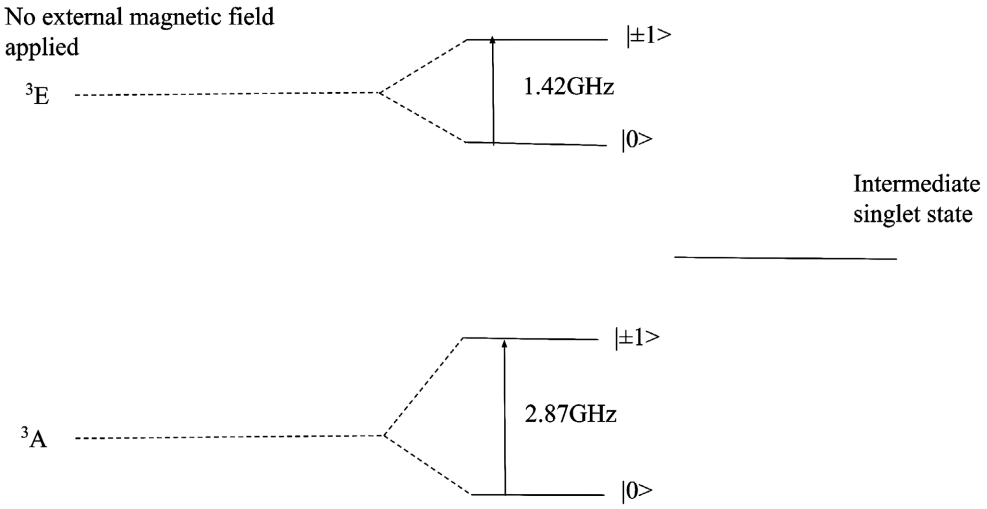

Figure 3. Energy level diagram of the energy states in the NV center without an external magnetic field.

place, where the |±1> states further split into |−1> and |+1> states, with the |+1> state at higher energy shown in Figure 4 [7]. The Zeeman splitting occurs because spins pointing in different directions (such as those of the $m = -1$ and +1 levels) gain or lose energy when they are parallel or antiparallel to the external magnetic field.

2.4. Detection of External Magnetic Field Strength with NV Centers

If a beam of green laser is directed to the NV center, the electrons would be optically pumped from the ground state to the high energy ^{3}E states. This is illustrated by Figure 5, they will be pumped to the ^{3}E |±1> states from ^{3}A |±1> if they

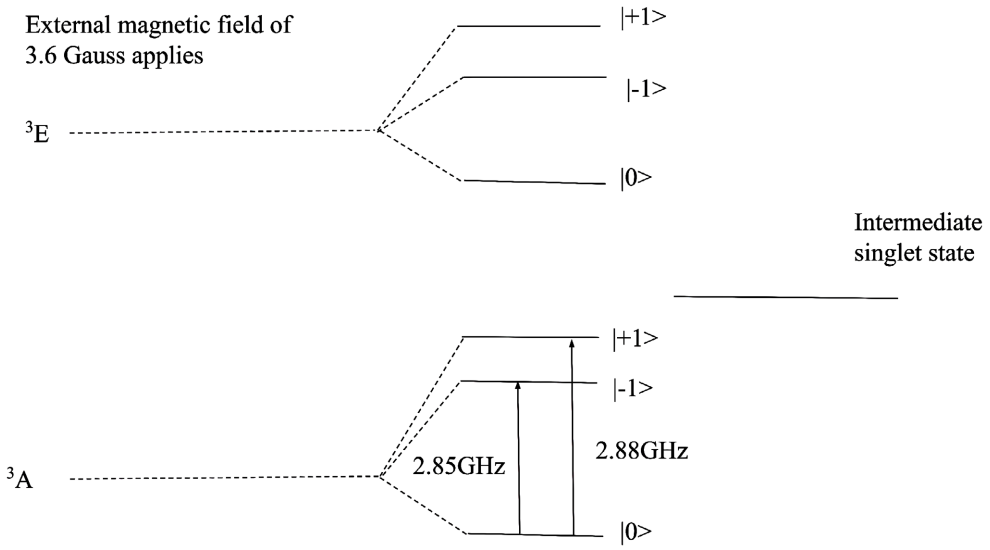

Figure 4. Energy level diagram of the energy states in the NV center with an external magnetic field.

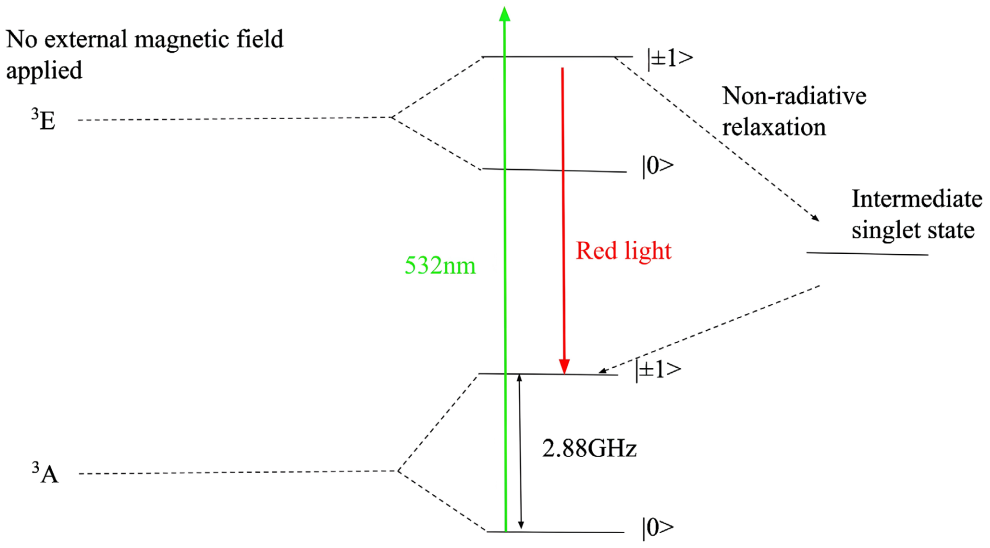

Figure 5. Process of the excitation of the electrons from ^{3}A |0> to ^{3}A |±1> with a microwave, then its excitation to ^{3}E |±1> state with a beam of green light, and the decay of the NV center back to ^{3}A |±1> state.

were initially at ^{3}A |±1>; they will be pumped to the ^{3}E |0> states from ^{3}A |0> if they were initially at ^{3}A |0>. These transitions are selective on the value of m because the spin is conserved upon photoexcitation [10].

2.5. Decay of the Electrons Back to Their Ground States

After being pumped to the higher energy states, the electrons would decay back to the ground state. The decay can be through 2 processes: 1) spin-conserving photon emission; or 2) non-radiative relaxation [8]. Spin-conserving photon emission means that electrons will emit photons, that is, light, hence there will be a fluorescence observed. Non-radiative relaxation means that electrons would decay back via the intermediate singlet state, in the process releasing heat (vibrations of the diamond lattice) and emitting no light. When the NV center is excited into the ^{3}E |0> spin state, the electrons in the NV center would decay by mainly the spin-conserving photon emission back to the ^{3}A |0> spin state, emitting a red fluorescence and some heat. When the NV center is at ^{3}E |±1> spin state, the electrons relax to the ^{3}A |±1> state non-radiatively with higher probability [8], emitting less fluorescence compared to when the NV centers decays from ^{3}E |0>. This is shown in **Figure 5**. The difference in the amount of fluorescence provides the optical contrast necessary to perform the so-called Optically Detected Magnetic Resonance (ODMR).

2.6. Optical Signaling of the NV Center

The emitted fluorescence is around 30% higher for the decay from ^{3}E |0> to ^{3}A |0> state than for the ^{3}E |±1> to ^{3}A |±1> states [7] [11]. Hence, there is quite a strong contrast that can be observed with regards to the fluorescence intensity.

Figure 6 shows the graph of intensity of fluorescence emitted as a function of the gigahertz supplied to the ^{3}E |0> state electrons, without and with an external magnetic field.

As seen from **Figure 6(a)**, when the microwave frequency applied to the NV center is 2.87 GHz, the intensity of the fluorescence detected dipped. This shows that the NV center decays from ^{3}E |±1> to ^{3}A |±1>, which means that the NV center is pumped from ^{3}A |0> to ^{3}A |±1> by 2.87 GHz.

2.7. Effect of External Magnetic Fields on the Optical Signal

If there is a magnetic field applied to this system, the Zeeman effect would take place [7], where the |±1> states further split into |−1> and |+1> states, with the |+1> state at higher energy. To increase the NV center from ^{3}A |0> spin state to ^{3}A |+1> spin state would now require a higher microwave frequency of around 2.88 GHz with reference to **Figure 6(b)**.

With 3.6 Gauss of external magnetic field applied to the setup in **Figure 6(b)**, the first dip in fluorescence is at about 2.86 GHz. When the microwave is applied at 2.85 GHz, the NV center would be pumped from the ^{3}A |0> state to the ^{3}A |−1> state. The green laser then sends the NV center up to the ^{3}E |−1> state, which

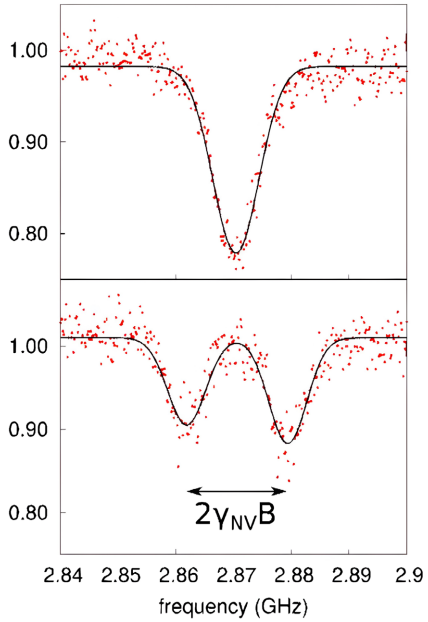

Fig 6a, Intensity of fluorescence detected without an external magnetic field

Fig 6b, Intensity of fluorescence detected with an external magnetic field of 3.6 Gauss

Figure 6. Optical signal to indicate the strength of the external magnetic field applied.

then decays back to the ^{3}E |−1> state via mainly the non-radiative relaxation method, causing the intensity of the fluorescence detected to dip.

The second dip in fluorescence is at about 2.88 GHz. When the microwave is applied at 2.88 GHz, the NV center would be pumped from the ^{3}A |0> state to the ^{3}A |+1> state. The green laser then sends the NV center up to the ^{3}E |+1> state, and then decays back to the ^{3}A |+1> state via mainly the non-radiative relaxation method, causing again the fluorescence detected to dip. The red arrow indicates the energy difference between the ^{3}A |−1> and ^{3}A |+1> states.

The larger the frequency difference indicated by the arrow in **Figure 6(b)**, the larger the energy difference between spin |−1> and spin |+1> states, hence the stronger the Zeeman effect and greater the external magnetic field applied. The magnetic field strength is directly proportional to the energy difference between the ^{3}A |−1> and ^{3}A |+1> states [10], providing a mechanism to spectroscopically and quantitatively measure the magnitude of the magnetic field, shown in **Figure 7**.

2.8. Spin Coherence Time

The spin coherence time is of significance for the detection of magnetic field strength. The spin states |0>, |−1> and |+1> are pure states. If the electron spins are not coherent, the NV center will not be in a pure spin state, but it would exist in multiple states at the same time (*mixed state*), so the signals detected would mix up, so sensitive and precise detection would not be possible. The spin coherence time of NV centers exceeds 400 μs at room temperature with dynamical decoupling [12], which is a relatively long coherence time compared to other quantum sensors. Therefore, using an NV center instead of other quantum sensors is advantageous. Other than that, its high spatial resolution and high sensitivity

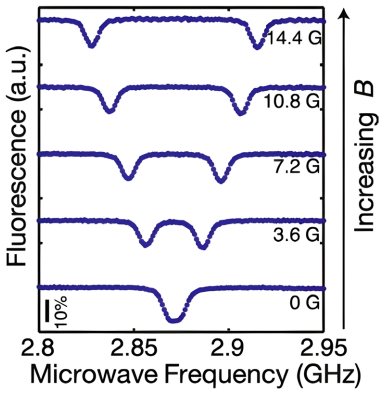

Figure 7. The effect of increasing the external magnetic field strength on the energy difference between the two microwaves.

will be helpful in understanding material properties [13], to discover new materials or enhance biomedical techniques including single-molecule detection.

3. Application and Outlook of NV Centers

Given the ability of NV centers to detect the strength of external magnetic fields, this quantum sensing technology can be applied into practical fields, including the identification of certain molecules or the study of superconductors under high pressure, or again the rising technology of Artificial Intelligence and Robotics.

3.1. Application of NV Center in the Study of Biotechnology and Medicine

NV centers can be used to carry out NMR from ten-picolitre volumes, which is from about 10^{-11} liters [14], to better understand and characterize organic and biological molecules and macromolecules (proteins, enzymes, etc.) including several of crucial importance for life science and biotechnology applications [15]. The high spatial resolution of NV centers [15] enables them to image biological samples with much higher resolution than MRI scanners. They can also reveal changes in chemical compositions from the micro to nano scale.

A thin diamond chip that is a few millimeters thick with a thin surface layer of NV ensembles, can be used to detect the magnetic fields produced by individual cells, enabling their identification. Since NV centers are highly sensitive to external magnetic fields but otherwise occupy a very small area, the image they produce has a high spatial resolution when they are scanned on an area of interest [15]. This is a new technology to diagnose cancer cells from normal cells. The problem with this method is that the cells may not always align to the N-V axis, and it is difficult to make them align to the axis. Hence, researchers insert nanodiamonds containing NV centers into the interior of cells or bacteria to better detect its magnetic properties and discover properties of cells or certain cancer biomarkers such as the presence of certain proteins [15].

NV centers are highly sensitive to magnetic noises at the NV spin transition frequency—it can be used to detect magnetic ions such as Gd^{3+} [15]. Gd^{3+} can

improve the clarity of the MRI image, by improving the visibility of inflammation, tumors and blood supply for some organs [16].

NV centers are highly sensitive to free radicals in tissues since free radicals have a large spin noise, due to the presence of an unpaired electron [17]. Hence, NV centers can be used to detect free radicals in the human body, which is highly related to cardiovascular diseases, neurological disorders, and the immune system.

3.2. Application of NV Centers in Studying Superconducting Materials

NV centers can further be used to study materials under high pressure [1], since under high pressure, some materials become superconducting, which makes them perfect diamagnets. This perfect diamagnetism (also known as the *Meissner effect*) produces a characteristic magnetic response to external fields. NV centers embedded in the high-pressure cells (which use diamond anvils [18]) can hence study the transition of a material from normal to superconducting state. In **Figure 8**, the 2 diamond anvils are exerting pressure on the material to transit it into its superconducting state.

NV centers can be inserted into the culet of the Diamond Anvils to detect the changes in magnetic properties of the material. This is to ensure that the distance between the NV center and the sample is as close as possible, to ensure the NV center can detect the magnetic field of the sample with maximum sensitivity (see also **Figure 9**). The "boxes" in **Figure 9** placed at the culets of the Anvils

Figure 8. Diamond anvil cell.

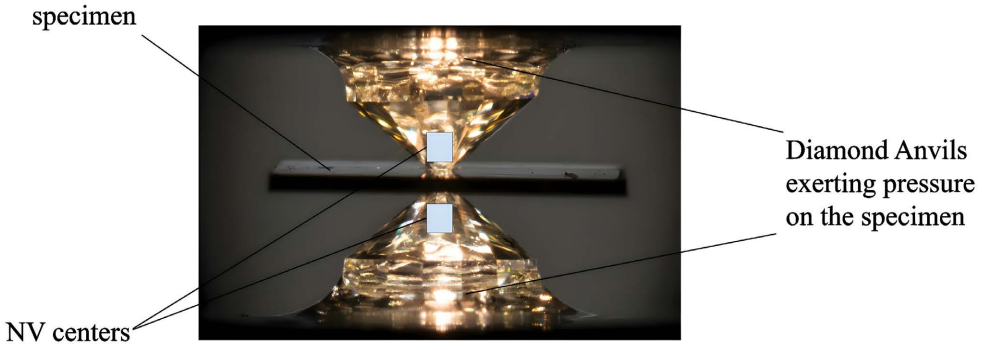

Figure 9. Diamond anvil cells with NV centers.

show where the NV centers are supposed to be placed at.

4. Conclusions

In conclusion, there is great potential in NV center-based quantum technologies, with several developments in multiple scientific and technological areas. The capabilities of NV centers to perform nanoscale measurements of magnetic fields and other observables and their exceptional sensitivity to external environments will enable them to revolutionize medical, neurological, robotic, and superconducting fields, and many other areas.

Although there are still challenges with regards to maximizing the capabilities of NV centers, such as improving their coherence time, the promise of NV centers as quantum sensors is undeniable. As research continues, we are on the edge of uncovering the immense potential of NV centers across numerous domains of science.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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