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NV^- center emulation in an external magnetic field

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Abstract. The work is devoted to emulating the correlation of a projection of magnetic field vector on axes of nitrogen-vacancy center in diamond lattice with frequencies of optically detected magnetic resonance (ODMR). The projection of the magnetic field on the axes, which reflect the bonds of the carbon atom vacancy with the neighboring carbon atoms and the nitrogen atom, is calculated in this work. The paper highlights the algorithmic representation of the above calculations by software. The dependence of the optically detected magnetic resonance on the direction and magnitude of the magnetic induction vector is demonstrated. In total, there are 4 bonds between the vacancy and neighboring atoms located at an angle of 109.5° relative to each other. Having the magnitude of the ODMR signal, it is possible to reconstruct the vector of the external magnetic field, taking into account its projection angle on the bonds with the vacancy.

Keywords: ODMR, external magnetic field, NV-center, axis, energy sublevel.

1. Introduction

An NV center is an impurity-defect complex in diamond, the electronic levels of which experience a fine splitting into spin states, which is caused by different mutual orientations of their half-integer spins. When a tetravalent carbon atom is replaced by pentavalent nitrogen, an additional electron appears in the lattice, and when a neighboring vacancy is formed, four more electrons are released. So, three valence electrons of the nitrogen atom are covalently bonded to nearby carbon atoms, two to the vacancy. Often these five electrons attached to the center are joined by a sixth electron from another nitrogen atom. Thus, the center can be either neutral or negatively charged. It should be noted that the paramagnetic ground state of a center with a strong electron spin polarization is inherent only in the NV^- form. The energy of the zero energy sublevel turns out to be less than the energies of sublevels –1 and 1 by 2.87 GHz. [1]. In total, there are 4 bonds between the vacancy and neighboring atoms (including a nitrogen one) located at an angle of 109.5° relative to each other [2]. Having the magnitude of the signal of optically detected magnetic resonance (ODMR), it is possible to reconstruct the vector of the external magnetic field, taking into account its projection angle on the bonds with the vacancy [3].

2. Theoretical part

When a carbon atom is knocked out of the crystal lattice of a diamond, a vacancy forms in its place, that is, a defect that behaves like an atom. In the presence of an external magnetic field directed along the N-V axis, the spin energy levels of the ground state of the NV center are split, which depends linearly on the magnitude of the magnetic field. Thus, depending on the orientation of the half-integer spin of valence electrons, we can get three states of the system: if the electron spins are opposite, then the state of the system will correspond to the conditional zero sublevel, if they are codirectional, then the sum of their spins will give a transition to the level minus one or plus one depending on the orientation of the spin. The designations of the sublevels correspond to the quantum magnetic number. If, in this case, an oscillating weak magnetic field is applied in the perpendicular direction in the form of microwave radiation of a certain frequency coinciding with the distance between the split energy levels, then the electromagnetic field quantum will be absorbed and the system will transition to a state with a higher energy with a change in the magnetic quantum number by unity (paramagnetic resonance).For a system of N particles in three dimensions, one energy level can correspond to several different wave functions. All these degenerate states at the same level can be filled with equal probability. The number of such states gives the degeneracy of one or another energy level. However, in the presence of a magnetic field, an electron with a magnetic moment acquires additional energy. The acquired energy leads to the removal of the degeneracy of atomic states in terms of the total quantum number and the decoupling of atomic spectral lines (the Zeeman effect).

The ground and excited states are connected by optical transitions with a wavelength of 637 nm, for which the selection rule $\Delta m_S = 0$ is satisfied. That is, the transition from the ground state to the excited state and vice versa occurs with the preservation of the spin projection, which means that the transition will be made to a similar sublevel, since both the ground and excited states experience splitting (Fig.1).

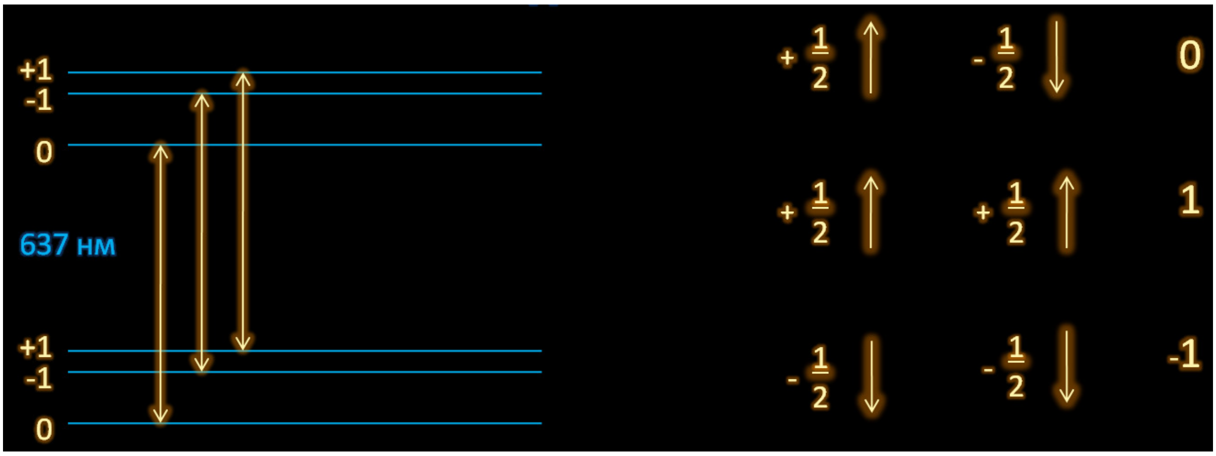

Fig 1. Splitting of the energy levels of the NV-center and their relationship with spin orientation.

After excitation by a laser, the system goes into an excited state, but after some time (~10 ns) it decays into the ground state. During the transition from the ground state to the excited state, absorption and emission of vibrational motion quanta occur. Upon transition to an excited state, phonons are emitted due to the energy imparted to the electrons and the electrons pass to the corresponding energy sublevel. The reverse transition occurs with the absorption of phonons. Also, during the radiative decay of an excited state, a fast nonradiative transition to an intermediate state first occurs, which then spontaneously decays into a metastable state [4]. Further, nonradiative relaxation occurs from this state to the ground state at the magnetic sublevel $m_S = 0$.

During the excitation of the system, the phenomenon of photoluminescence is observed, and depending on the intensity of the field effect on the N-V bond, the intensity of photoluminescence can also change. After exposure of the system to a microwave field, the photoluminescence index begins to drop sharply. The microwave field excites +1 and –1 sublevels and with a probability of 15-20% a side channel of relaxation appears. In this case, energy is spent on the processes associated with relaxation and the intensity of photoluminescence decreases. The ratio between the photoluminescence index in the absence of a microwave field and the photoluminescence index with the presence of a microwave field is called contrast. Near the frequencies corresponding to the frequencies of finding sublevels +1 and –1, the contrast begins to increase [1].

Depending on the projection of the magnetic field vector on the N-V axis, different frequency indices can be observed, in which the maximum contrast is achieved.

In other words, if the magnetic field is directed at some angle to the N-V axis, we can observe the frequency detuning at which the –1 and +1 sublevels are located. In the case of a complex of NV centers, we can see several peaks on the graph of the dependence of the contrast value on the radiation frequency for different projections on different N-V axes. For example, in the case of a complex of two nv-centers with a different projection of the external magnetic field vector on the N-V bonds, we will get different detunings, two for each axis. Thus, the maximum possible number of peaks for a complex of two NV centers is four. If the projections match, the detuning values will match. It is also possible that the deviation of the vector by some angle from the state of coincidence of the detuning values will give only one additional peak. ODMR phenomenon of optically detected magnetic resonance, during which there is an increase in the contrast between the photoluminescence index in the absence of a microwave field and the photoluminescence index with the presence of a microwave field and a detuning of resonant frequencies corresponding to +1 and –1 sublevels.

3. Geometric representation and calculations

For convenience, let us imagine a fragment of a unit cell of the diamond crystal lattice, containing an NV center, enclosed in an abstract cube (Fig.2). Suppose the magnetic induction vector always falls perpendicular to the xz plane, and all mutual positions of the lattice and the vector are expressed by manipulating the position of the crystal lattice. In turn, any position of the crystal lattice can be expressed through its rotations along the X, Y, Z axes. Figure 3 shows that the decision to rotate the NV center relative to the static vector is similar to the rotation of the vector relative to the static NV center.

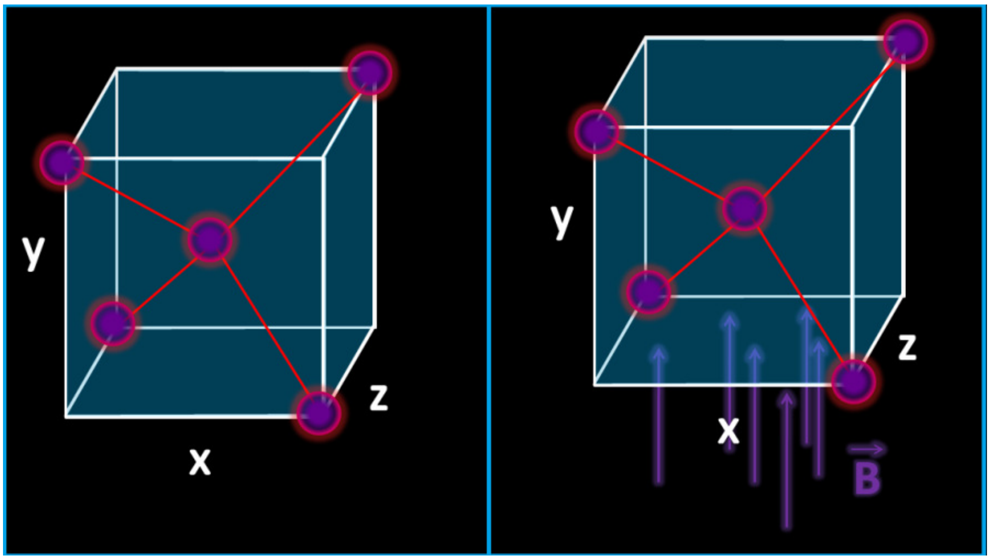

Fig.2. On the left is a fragment of a unit cell of a crystal lattice with an NV center. Right-effect of a magnetic field on the NV center perpendicular to the XZ plane.

Calculations are made according to the formula:

$$v(B_z) = D \pm \sqrt{g \cdot m \cdot \frac{B_z}{h} + E^2}\ , \qquad (1)$$

where D = 2.87 GHz is the axial splitting parameter in zero external field, g ~ 2 is the Lande coefficient for vacancy electrons, h is the bar constant, E is the off-axis splitting parameter in zero field, B_z is the projection of the magnetic evaluation vector, v is the frequency of sublevels + 1 and – 1, m is the Bohr magneton.

Consider the axis of one NV center. The first column contains the rotation angles, the first row contains the rotation angles, the second row contains the rotation angles, the second row contains the y-axis, and the third row contains the z-axis. In the fourth line of the first column – the value of the supplied magnetic field vector. The second column characterizes the projection on the axis as a percentage. The first line contains the percentage projection on the NV center for this model. The third column contains the projection from the input vector. The projection to the N-V axis is also in the first line. In the last column we see the detuning values, that is, the values for the frequencies at which the sublevels are now located (Table 1). When rotated 30 degrees in the x-axis and 5 degrees in the y-axis, we get:

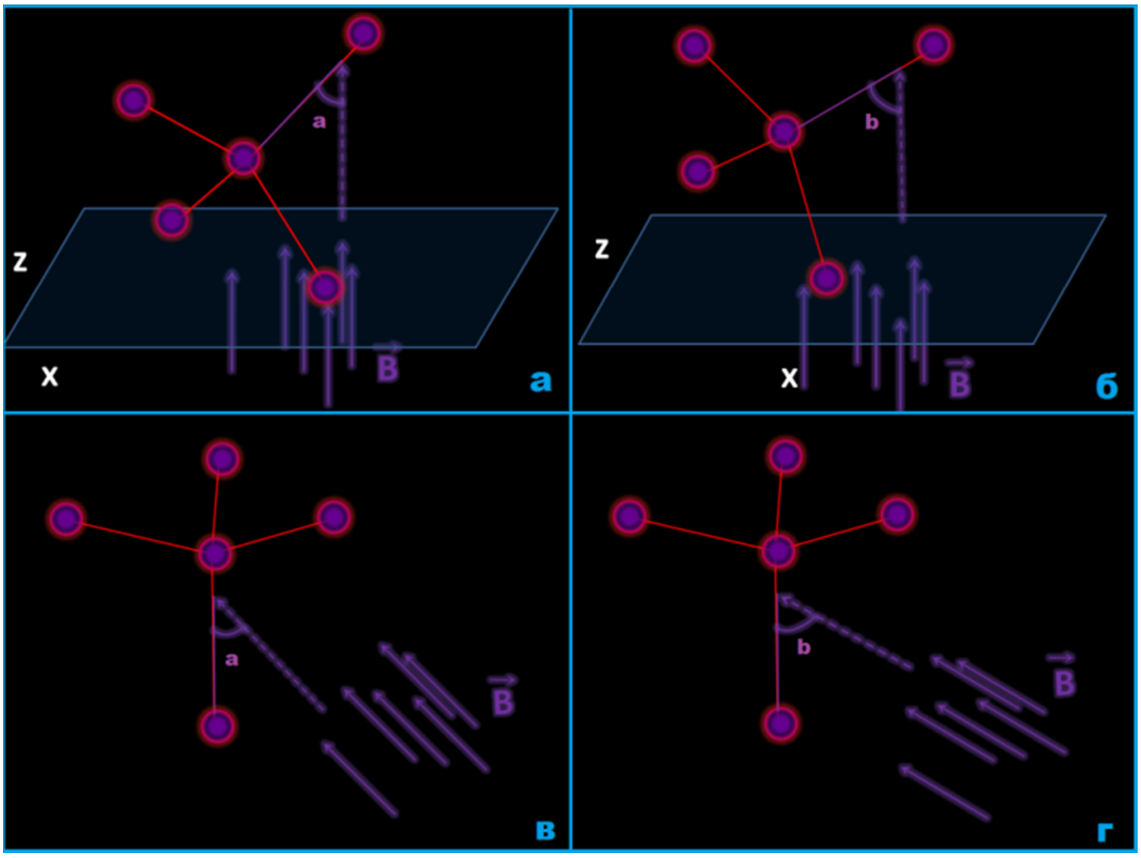

Fig.3. In figure a, the NV-center is located at an angle a, in figure b at an angle b relative to the magnetic induction vector. As can be seen from figures c and d, the transformations of the angle of the magnetic induction vector are similar to the rotation of the NV center relative to the latter.

Table 1. Detuning frequency values after changes

Input parameters	Percentage projection	Projection of the magnetic induction vector, G	Detuning frequency, GHz
30	0.8765	13.1477	2.9074
5	0.7517	11.2756	2.8336
0	0.7517	11.2756	
15	0.8765	13.1477	

Let's say that we have a complex of 4 NV centers whose axes do not coincide, which means that the maximum possible number of peaks is eight. Since the complex of NV centers is mutually connected, the projections on similarly located axes will coincide during the rotation of such a system. That is, in fact, the system has 4 different options for the location of N-V axes in accordance with the number of links. Suppose that in the complex all the axes are located differently. By exposing the N-V bonds to a magnetic field of various magnitudes from the side of the XZ plane, we get:

Table 2. Sublevel detunings are now lined up in columns 4 and 5, two for each axis

Input parameters	Percentage projection	Projection of the magnetic induction vector, G	Detuning frequency of sublevel +1, GHz	Detuning frequency of sublevel -1, GHz
0	0.8165	32.6599	2.9619	2.7791
0	0.8165	32.6599	2.9619	2.7791
0	0.8165	32.6599	2.9619	2.,7791
40	0.8165	32.6599	2.9619	2.7791

If we rotate the system 30 degrees around the axis and 30 degrees around the z-axis, we get:

Table 3. Projection values for each axis are not repeated

Input parameters	Percentage projection	Projection of the magnetic induction vector, G	Detuning frequency of sublevel +1, GHz	Detuning frequency of sublevel -1, GHz
30	0.8682	12.1550	2.9046	2.8364
0	0.7404	10.3656	2.8996	2.8414
30	0.8834	12.3669	2.9052	2.8358
40	0.7644	10.7022	2.9005	2.8405

As we can see, in this system, the offset frequencies are completely different, so we get all 8 peaks.

4. Conclusion

Depending on the projection of the magnetic field vector on the N-V axis, the resonant frequencies may vary. Since each N-V axis corresponds to two peaks of maximum contrast, for a complex of k NV centers, this number will usually multiply by a factor, giving a maximum of $k\times2$.The algorithm for calculating the dependence of the frequency detuning value on the value of the projection vector on the axis of the NV center can be implemented in software. The computational part is reduced to software-implemented solutions of geometric problems, in other words, the calculation of the ODMR value in this case falls under the tasks of mathematical modeling.

Acknowledgements

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5. References

[1] Tsukanov, A.V., *Microelectronics*, **41**(2), 104, 2012; doi: 10.1134/S1063739712020084
[2] Novokreshchenova E.P., *Introduction to Crystal Chemistry of Semiconductors: Textbook*, (Voronezh: FGBOU VPO "Voronezh State Technical University", 2012). [in Russian]
[3] Neumann P., et al., *New J. Phys.*, **11**, 013017, 2009; doi: 10.1088/1367-2630/11/1/013017
[4] Acosta V.M., Jarmola A., Bauch E., Budker D., *Phys. Rev.*, **82**, 201202R, 2010; doi: 10.1103/PhysRevB.82.201202