Definition of the NV-center orientations relative to the diamond crystal plane

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Abstract. We investigate the electron spin resonance of an ensemble of Nitrogen-Vacancy color centers in a bulk diamond crystal obtained by CVD-method. The diamond crystal had 1 ppm concentration of nitrogen. The four possible orientations of the NV-center in the crystal lattice lead to different dependences of a magnitude and an orientation of the external static magnetic field. We used the field of 35 Gauss with the vector in the plane of the crystal. We could rotate it to a certain angle within almost 360 degrees around the normal vector to the plane of the crystal. The goal was to define the unknown orientations of the four axes of the NV-centers relatively to the crystal plane. Experimental results obtained at room temperature with a continuous microwave excitation and presented in this paper are in a good agreement with our simulations.

The electron spin in Nitrogen-Vacancy (NV) color centers in diamond crystals is a solid-state qubit [1], suitable for use in various fields of quantum information technologies, and allows high-precision measurements of magnetic fields on the nano-scale. Due to the C₃ᵥ symmetry of NV centers [2], each defect in diamond has four possible orientations in the crystal lattice [3]. In the framework of this work, we studied a diamond sample with a large ensemble of NV centers.

In the general case, due to inaccuracies in processing the surface of a diamond sample and inhomogeneity of the external magnetic field, the orientation of the axes of the NV centers relative to the external magnetic field is unknown or known with a limited accuracy [4].

To solve this problem, we studied an influence of an external magnetic field on the resonant behavior of the electron spin in NV centers in the diamond at room temperature. The photoluminescence intensity of the NV center was measured as a function of a frequency of the microwave field in optically detectable magnetic resonance (ODMR) using an external magnetic field [5]. The direction of the external constant magnetic field must be parallel to the crystal axis so that there is a maximum splitting mₛ = ± 1 of the energy levels of NV centers for this particular axis in the diamond crystal. The 35 G external magnetic field vector was in the plane of the diamond crystal and could be rotated around the plane at any angle within almost 360 degrees. The vector of the microwave magnetic field with a frequency of about 2.87 GHz was perpendicular to this plane. The results of experimental measurements are compared with the results of a theoretical simulation.
A CVD bulk diamond crystal has been taken as an object of investigation. The concentration of Nitrogen-Vacancy color centers in the bulk was about one ppm. A laboratory setup based on confocal microscope to determine the orientation of the axes of the NV centers [6] has been used. In addition, the violation of spatial symmetry was achieved by introducing a constant external magnetic field in the plane of the crystal surface with the possibility of rotating it at a given angle around the plane of the crystal.

According to the diamond crystal structure there are four directions of the axes of NV-centers.

In the Cartesian coordinates (figure 1) these directions are given by vectors:

\[
\begin{align*}
C_1 &= (0 \ 0 \ 1)^T, \\
C_2 &= \left(\frac{2\sqrt{2}}{3} \ 0 \ -\frac{1}{3}\right)^T, \\
C_3 &= \left(-\frac{\sqrt{2}}{3} \ \frac{\sqrt{2}}{\sqrt{3}} \ -\frac{1}{3}\right)^T, \\
C_4 &= \left(-\frac{\sqrt{2}}{3} \ -\frac{\sqrt{2}}{\sqrt{3}} \ -\frac{1}{3}\right)^T.
\end{align*}
\]

(1)

When the NV centers are excited by a laser with a wavelength of 532 nm changes of the microwave radiation frequency causes shifts in the luminescence intensity decrements (the contrast of the ODMR). These observed shifts from the central frequency of 2.87 GHz are proportional to the projections of the external magnetic field on the axes of the NV-centers [7].
Figure 2 shows the ODMR contrast changes at the initial position of the external static magnetic field relative to the crystal surface (the rotation angle is zero).

Likewise, we obtained the changes of the luminescence under the influence of the microwave radiation with a constant external magnetic field rotated around the normal to the crystal surface at angles from 10° to 350° with a step of 10°. For the sake of convenience, the experimental data of the contrast changes are shown in figure 3 in the form of loops. Blue color indicates areas with the maximum luminescence decrease when exposed to microwave radiation, and yellow color indicates areas without luminescence decrease. The light blue color shows the intermediate areas.

By means of mathematical modeling, we found the relative angular position between the axes of the NV centers and the normal vector to the plane of the crystal. Since normal vector was the axis of the external magnetic field rotation, we found it as the following vector in Cartesian coordinates shown in figure 1:

\[
\mathbf{M} = (-0.43, 0.77, 0.47)^T.
\]

Figure 4 shows the location of the rotation axis of the external magnetic field. To clarify the distortions caused by the projection of the three-dimensional image onto the plane, it should be explained that the vector \( \mathbf{M} \) lies practically in the plane formed by the vectors \( \mathbf{C}_1 \) and \( \mathbf{C}_3 \).

Figure 5 shows the calculated trajectories of luminescence minima as the external magnetic field rotates around the \( \mathbf{M} \) axis. The trajectories of the minima caused by the changes in the projections of the external magnetic field onto the directions \( \mathbf{C}_1, \mathbf{C}_2, \mathbf{C}_3 \) or \( \mathbf{C}_4 \) during the rotation of the magnetic field.
around the M axis are colored as corresponding directions on figure 1. For clarity, the trajectories were imposed on the experimental data shown in figure 3.

![Figure 5](image_url)  
**Figure 5.** Calculated trajectories of changes in the ODMR signal during the rotation of an external magnetic field.

Thus, using the experimental data, we have successfully determined the orientation of the axes of NV-centers relative to the rotation axis of the external magnetic field, which matches the normal to the crystal surface.

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