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The influence of diamond origin on the properties of NV centers

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Abstract. Diamond samples of various origins containing NV centers were studied using optically detected magnetic resonance (ODMR) and photoluminescence (PL) methods. It is shown that various impurities and deformation-induced defects can significantly influence the crystal environment and properties of NV centers. This influence is reflected in such characteristics as the distribution of NV centers throughout the crystal volume, their charge state (the ratio of neutral to negatively charged NV centers), mechanical stresses and strains in their crystalline environment, interaction with a nitrogen donor, which affects their coherent properties, and their orientation within the diamond lattice.

Keywords: diamond, photoluminescence, optically detected magnetic resonance, NV center, scanning confocal microscopy

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Влияние происхождения алмаза на свойства NV-центров

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Аннотация. Методами оптически детектируемого магнитного резонанса (ОДМР) и фотолюминесценции (ФЛ) были исследованы образцы алмазов различного происхождения, содержащих NV-центры. Было показано, что различные примеси и деформационные дефекты могут оказывать значительное влияние на кристаллическое окружение и свойства NV-центров. Это влияние отражается в таких характеристиках, как распределение NV-центров по объему кристалла, их зарядовое состояние (соотношение нейтральных NV-центров к отрицательно заряженным), механические напряжения и деформации их кристаллического окружения, взаимодействие с донором азота, влияющим на их когерентные свойства, и их ориентация в алмазной решетке.

Ключевые слова: алмаз, фотолюминесценция, оптически детектируемый магнитный резонанс, NV-центр, сканирующая конфокальная микроскопия

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Introduction

Diamond is a highly promising mineral with a wide range of industrial and technological uses. Particular attention is paid to the well-known NV center, one of its paramagnetic defects. It represents a negatively charged center consisting of a substitutional nitrogen atom bound to a carbon vacancy. Optical excitation of NV centers leads to optically induced alignment of the electron populations of the spin sublevels of the ground triplet state, resulting in the filling of the spin sublevel with $M_S = 0$, opening the possibility of spin manipulation using ODMR [1–3].

The spin Hamiltonian describing the NV center ODMR spectrum (excluding quadrupole interactions with nitrogen and hyperfine interaction with ligands of ^{13}C) has the form [4]:

$$H = \mu_B g_e \mathbf{S}\cdot\mathbf{B} + D\left[S_Z^2 - \frac{1}{3}S(S+1)\right] + E\left(S_{1X}^2 - S_{1Y}^2\right) + \mathbf{S}\cdot\mathbf{A}_{\mathbf{NV}}\cdot\mathbf{I}_{\mathbf{N}}, \quad (1)$$

where the first term describes the electronic Zeeman interaction, the second and the third terms describe the NV^- center zero field splitting (ZFS), $S = 1$ is the spin of the NV^- center, S_X, S_Y, S_Z are the projections of the spin S onto the coordinate axes X, Y, and Z, respectively; the parameter $D = 2870$ MHz describes the axial part of ZFS; the parameter $E = 0$–20 MHz describes the non-axial part of ZFS and depends on stress and strain in the diamond sample; $\mathbf{A}_{\mathbf{NV}}$ is the anisotropic ^{14}N hyperfine structure interaction parameter for the NV^- center, which is axially symmetric with respect to the symmetry axis of the NV^- center, that is directed along one of the four ⟨111⟩ axes of a diamond. The spin Hamiltonian parameters are key for the for the interpretation of the experiments, since they directly influence the ODMR spectrum shape, which allows extracting information about the NV^- centers local environment, which depends on the diamond sample origin and treatment.

Since the NV center is sensitive to changes in external conditions, such as magnetic and electric fields, temperature, pressure, stresses and strains, it can be used as a probe for local visualization and diagnostics of diamond properties in its environment. Therefore, the aim of this work is to study the diamonds of different origin, containing NV centers, in order to investigate their internal structure and the effect of the crystalline environment on the properties of NV centers.

Materials and Methods

In this study a home-made ODMR spectrometer equipped with a confocal optical circuit (NT-MDT SI) was used [5, 6]. It allows registration of PL and ODMR signals in the region of ~1 μm in diameter at room temperature. It is possible to reveal the spatial distribution of PL and ODMR signals using confocal 3D (X, Y, Z) scanning with a micron resolution. The following instrumental setup was used: objectives (×100 and ×10) and pinhole with diameter from 100 μm, lock-in detector, low-frequency generator, microwave generator working in the range of 2–4 GHz with an antenna for feeding of resonant microwave power to the sample, CCD camera for recording the PL spectra, PMT for ODMR registration. The PL was excited by a laser with a wavelength of 532 nm and a power of $P = 5$ mW. The ODMR spectra of NV^- centers were obtained by lock-in detection of changes in the PL intensity under conditions of magnetic resonance with microwave frequency sweep at the frequency of amplitude modulation of microwave power 680 Hz. ODMR was recorded in the zero-phonon line (ZPL) and phonon sideband (PSB) regions of the NV^- center.

Studies were carried out on six samples belonging to the different groups of diamonds, containing NV centers [4], at room and liquid nitrogen temperature:

1) Natural plastically deformed cubic diamond of the variety II [7] (sample *1*), belonging to type IaA + Ib.

2) Treated natural type IIa diamond (~1 ppm of N impurity) (sample *2*). NV centers were artificially created via fast neutron irradiation (~10^{18} cm^{-2}) and annealing at 800 °C for 1 hour.

3) Synthetic HPHT diamond with high nitrogen (~300 ppm of N impurity) (sample *3*), irradiated by either electrons or neutrons (10^{18} cm^{-2}) and annealed at 800 °C to form NV centers.

4) Natural diamond cryptocrystalline aggregate (Orlov's variety X–carbonado [7]) (sample *4*) of micron-sized grains.

5) Natural diamond cryptocrystalline aggregate, carbonado (sample *5*), similar to sample *4* but containing native metal inclusions.

6) HPHT sintered aggregate of detonation nanodiamonds (6 GPa, 800 °C) (sample *6*).

The choice of research methods for each sample was determined by the objectives. Confocal photoluminescence (PL) scanning was performed for samples *1*, *2*, and *4*, as it is most effective for visualizing the spatial distribution of NV centers depending on the crystallization conditions of the diamond, as well as post-crystallization processes. PL spectra were measured for samples *2*, *4*, and *5*, demonstrating differences in the charge state of the centers, which is important for analyzing the influence of impurities. The ODMR study focused on the samples most representative for studying the influence of nitrogen concentration (samples *2* and *3*) and the textural features of the aggregates (samples *4* and *6*). This approach allowed for the most efficient identification of key patterns linking the origin of the diamond to the properties of the NV centers.

Results and Discussion

Distribution of NV centers in diamond crystals. The results of a natural plastically deformed diamond single crystal (sample *1*) study showed that NV centers are predominantly formed in dislocation slip planes (Fig. 1, *a*). In the treated diamond (sample *2*), NV centers are fairly uniformly distributed, without any patterns (Fig. 1, *b*). In natural cryptocrystalline diamond aggregate (sample *4*) NV centers distribution has the form of halo clusters (Fig. 1, *c*).

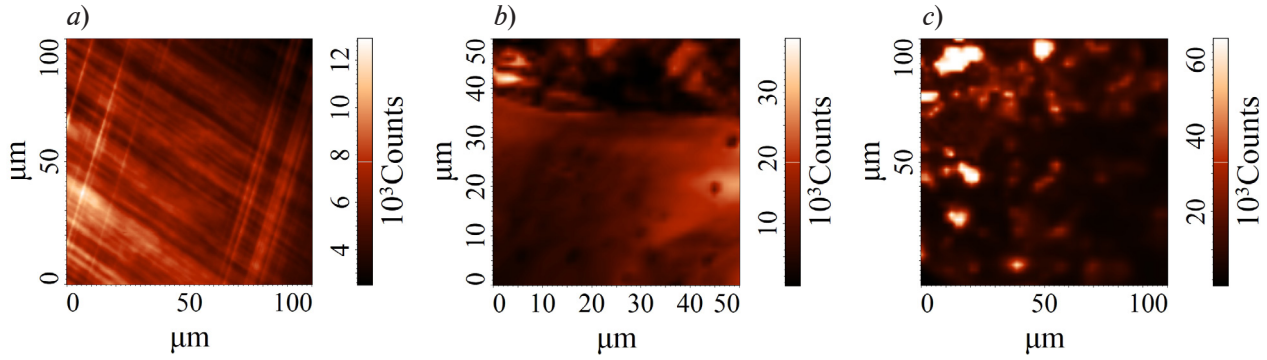

Fig. 1. PL scans of samples *1* (*a*), *2* (*b*) and *4* (*c*)

Fig. 2 shows the PL spectra of treated diamond and two carbonado samples (samples *2*, *4* and *5*, respectively). It can be seen that sample *4* has the lowest NV^0/NV^- ratio, less than 10%. This ratio can be measured by approximating the PL spectrum with a weighted sum of the reference spectra of NV^0 and NV^- centers. Furthermore, the PL spectrum of sample *4* does not contain any additional lines in contrast with PL spectra of samples *2* and *5*. Other defects in diamond can convert the negatively charged NV center into a neutral state [8].

Fig. 3 shows the ODMR spectra of samples *2* and *3*. Sample *2* has an extremely low nitrogen donor concentration, which can be seen in the ODMR spectrum, which has weak satellite lines and additional splitting of the central line caused by the NV center hyperfine structure. The local nitrogen donor concentration can be measured by calculating the intensity ratio of the satellite line to the central line [9]. For comparison, the ODMR spectrum of HPHT diamond (sample *3*), which has a high concentration of nitrogen donors (~300 ppm), is

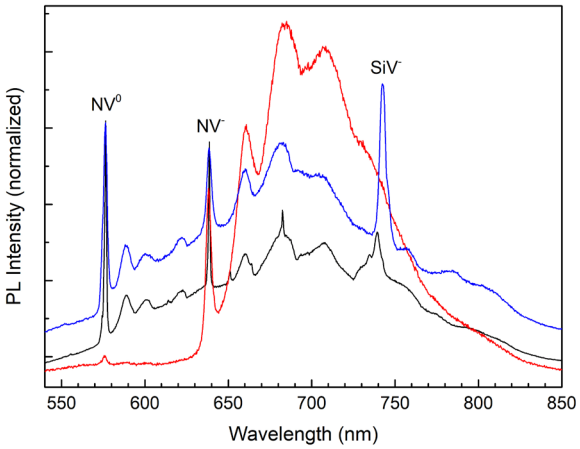

Fig. 2. PL spectra of samples *2* (black line), *4* (red line) and *5* (blue line), recorded at $T = 77$ K

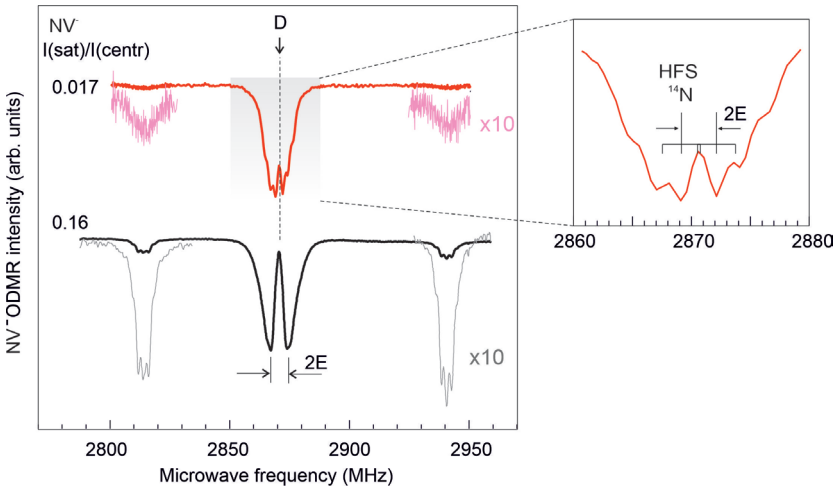

Fig. 3. ODMR spectra of samples *2* (red line) and *3* (black line); the inset shows an enlarged fragment of the sample *2* ODMR spectrum, where additional splitting of the central line can be seen

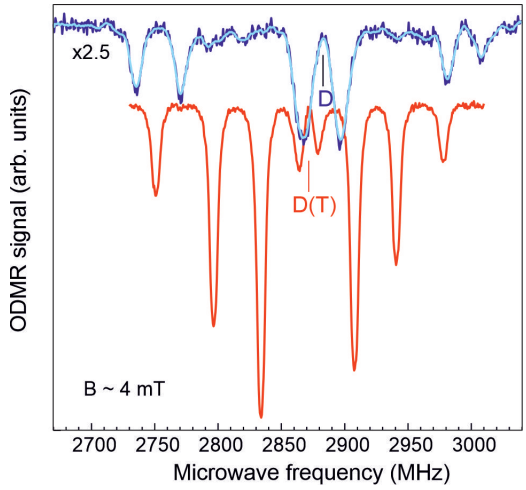

Fig. 4. ODMR spectra of samples *4* (blue line) and *6* (red line) with an additional magnetic field of ~ 4 mT directed at an arbitrary angle

shown. The intensity ratio of the satellite and central lines is more than 10%. The satellite lines also exhibit additional splitting due to the weak hyperfine interaction between the substitutional nitrogen atom and the nitrogen nucleus in the NV center.

Fig. 4 shows the ODMR spectra of carbonado and diamond aggregate obtained by HPHT sintering (samples *4* and *6*) with an additional magnetic field of ~4 mT directed at an arbitrary angle. It can be seen that the ODMR lines of sample 6 are better resolved, which can be explained by the same orientation of diamond crystals in the composition of sample *6*. The shift of its spectrum is associated with a temperature difference between samples *4* and *6*.

Conclusion

The characteristics of diamonds containing NV centers, such as the distribution of NV centers, their charge state, their interaction with nitrogen donors and their orientation in diamond, are highly dependent on the nature of each diamond origin and the way of NV centers formation.

In natural single crystals (sample *1*), the centers are localized along dislocation slip planes, reflecting their plastic deformation. In artificially irradiated crystals (sample *2*), the distribution is uniform, while in cryptocrystalline aggregates (sample *4*), it has a clustered character, reflecting their polycrystalline nature. The predominance of the negatively charged state of the NV centers over the neutral state is most pronounced in samples with minimal impurity and defect content (sample *4*). The presence of foreign defects, either naturally occurring (sample *5*) or by irradiation (sample *3*), facilitates the transition of the centers to the neutral state. The contrast and shape of the ODMR lines respond to the concentration of paramagnetic nitrogen (samples *2* and *3*), as confirmed by hyperfine structure analysis. The orientational ordering of crystallites in sintered aggregates (sample *6*) results in better resolution of the ODMR spectra compared to unoriented ones in natural aggregates (sample *4*).

Thus, the origin of the diamond and its treatment determine the morphology, charge state and spectral properties of NV centers, which allows them to be used not only as quantum sensors, but also as effective probes for diagnosing the internal structure and history of diamond materials of various natures.

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