Hyperfine and quadrupole coupling in hexagonal boron nitride

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Hexagonal boron nitride (hBN) has emerged as a prospective platform for quantum technologies owing to unique spin, optical and coherent properties. hBN offers a significant advantage for quantum applications by enabling the initialization, manipulation, and readout of spin states at room temperature — unlike superconducting qubits, which require cryogenic temperature [1–2]. Additionally, the hyperfine and quadrupole interactions between the electron spin of vacancies and nearby nuclei (^{10}B, ^{11}B and ^{14}N), allow the utilization of nuclear qubits as long-lived quantum memory units. This is critical for quantum devices, as nuclear spins exhibit millisecond-scale coherence times, ensuring robust information storage, while electron spins facilitate fast control and readout [3–4]. Therefore, boron vacancy centers in hBN, coupled with surrounding nuclear spins enable coherent multiqubit operations and quantum sensing applications. Understanding hyperfine (HFI) and quadrupole interactions (QI) in these systems crucial for advancing quantum computing and sensing protocols.

A high-purity hBN crystal ($0.90 \times 0.54 \times 0.05$ mm³) was irradiated with 2 MeV electrons to create boron vacancies. Electron paramagnetic resonance (EPR) measurements were performed at 94 GHz (W-band) using a Bruker Elexsys E680 spectrometer under optical excitation (λ = 532 nm). Pulsed electron-nuclear double resonance (ENDOR) at T = 25 K was employed to obtain signals arising from electron-nuclear interactions.

The boron vacancy spin system (S = 1) exhibited a zero-field splitting parameter D = 3550 MHz (T = 25 K) and g – factor = 2.004. For nitrogen nuclei ^{14}N (I = 1, 99.6 %) located closest to the spin defect were determined the HFI tensor components as A_{xx} = 46.5 MHz, A_{yy} = 45.0 MHz, A_{zz} = 87 MHz, with a quadrupole coupling constant C_q = 1.96 MHz and asymmetry parameter η = −0.07. The following parameters for ^{11}B nuclei (I = 3/2, 80.1%) in the second coordination sphere were also established: the hyperfine interaction tensor component A_{xx} = −3.80 MHz and the quadrupole coupling constant C_q = 2.7 MHz.

This work provides insights into the nuclear spin environment surrounding boron vacancies, specifying key parameters for optimizing quantum memory protocols and multi-qubit operations. The HFI and QI parameters determined in this work enable implementation of highly selective resonant transitions for pre-selected nuclei within the coordination sphere through narrow-band excitation pulses. Our findings directly contribute to the development of practical quantum computing architectures with application the unique advantages of two-dimensional materials for scalable quantum information processing.

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