Modelling Of The Quantum Response Of A Diamond-based NV Probe Chip For Biomedical Applications

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Abstract

This work presents the design and modelling of a quantum sensor based on the NV (Nitrogen-Vacancy) defect in the diamond lattice for in vitro biomedical applications. The platform employs ~150nm HPHT (High Pressure High Temperature) diamond nanoparticles (NDs) containing NV centers, surface-functionalized to bind directly to TRP (Transient Receptor Potential) channels on the membrane of neural cells. These temperature-sensitive ion channels are key pharmacological targets implicated in chronic pain, axonal neuropathy, lower urinary tract disorders, and type 2 diabetes. To support cell viability and enable quantum sensing, the system incorporates an indium tin oxide (ITO) heater for temperature control and a microwave (MW) antenna for resonant excitation of NV defects—both previously designed and numerically optimized in our earlier work. The NDs are dispersed in a small water reservoir that represents the biological medium surrounding the neural cell sample. Quantum sensing is based on the spin-dependent photoluminescence of the NV center, which enables sub-cellular temperature mapping with a theoretical sensitivity of 10 mK/√Hz.

This work builds directly upon our previous chip design by extending the model to include the quantum response of NV centers under dynamically varied thermal conditions in a liquid biological environment. In the first stage, we use COMSOL Multiphysics 6.3 with the heat transfer module and MATLAB LiveLink to simulate localized heating caused by laser absorption. The aim is to determine suitable laser wavelengths and powers capable of raising the local temperature to ~40 °C to mimic inflammation-induced activation of TRP channels. In the second stage, the thermal simulation results are used to calculate the quantum response of the NV center. A temperature-dependent spin Hamiltonian of the NV ground state is constructed, and its eigenvalues are used to reconstruct the expected optically detected magnetic resonance (ODMR) spectra under varying local conditions.

In conclusion, we present a fully modelled system for probing temperature in vivo in applications using nanodiamond-based quantum sensors in a controlled liquid environment. This work advances the design of NV-based nanoprobes for biomedical sensing and paves the way for future quantum diagnostic and therapeutic tools.