RF Magnetic Field Simulation of a Novel Planar DNP-NMR Coil

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Abstract

INTRODUCTION:
Nuclear magnetic resonance (NMR) spectroscopy is a broadly used research technique that exploits the magnetic properties of atomic nuclei with non-zero spin in order to determine the physical/chemical properties of the molecules in which they are contained. However, NMR has fundamental sensitivity limitations, as a consequence of the small energy difference between nuclear spin states.

To this end, dynamic nuclear polarization (DNP) has emerged as a widely applicable technique to improve the sensitivity of NMR experiments (RF currents typically of few hundreds of MHz) by transferring the relatively large polarization of electron spins to bulk nuclei, a process which requires the excitation of electron paramagnetic resonance transitions with high-power millimeter-wave (MMW) radiation (typically few hundreds of GHz). The result is a significant enhancement of the original NMR signal, thus leading to an important reduction of the corresponding spectrum acquisition times [Refs. 1,2].

In this paper, we develop a 3D simulation model in order to analyze the RF performance of a planar DNP-NMR coil, designed for room temperature experiments with liquid samples. The top part of the structure (Figure 1) is a wire grid polarizer, which serves in filtering out the polarization of the impinging MMW radiation. In what follows, we only deal with the RF performance of the circuit [Refs. 3-5].

USE OF COMSOL MULTIPHYSICS®:
The simulations are performed with the AC/DC Module of COMSOL Multiphysics® software, and in particular within the Magnetic Fields physics interface. A fully parametric model has been developed based on the 3D Inductor tutorial in the model library. The conductivity of copper is assigned to the coil surfaces via the use of an appropriate impedance boundary condition, while a lumped port is employed to feed in the circuit with a constant current of 1[A], as an approximation of a coaxial connector mounted on the left part of the structure. We are mainly interested in the surface current distribution on the surface of the coil, the magnetic field variation, and the average magnetic field over the sample volume.

RESULTS:
In the results, we vary only the angle of the tapered section on the left of the grid, to evaluate its effect on the field homogeneity in the sample region. The surface current distribution (Figure 2) highlights the regions where may cause inhomogeneities close to the sample, like around the two vertical holes used for injecting the liquid samples in the sample region. The variation of the magnetic flux density along characteristic lines of the geometry (Figure 3) suggests that a longer tapered section leads to a more homogeneous distribution, but at the cost of a lower volume-averaged value (Figure 4). Parameters that also have an important effect on these values are the periodicity of the wire grid as well as its distance from the bottom copper plate.

CONCLUSION:
This novel planar structure can be used as an efficient DNP-NMR coil, promising to significantly reduce the problem of excess heating of liquid samples at room temperatures.

Reference

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Figures used in the abstract

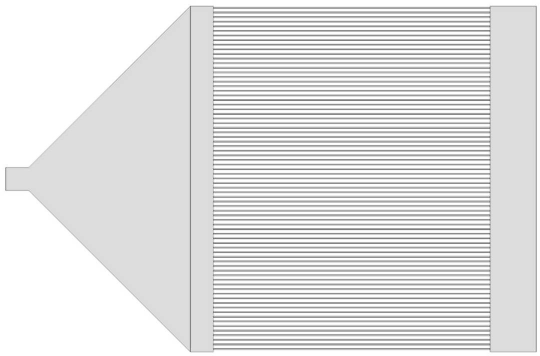

Figure 1: Top-view of the MMW grid polarizer geometry

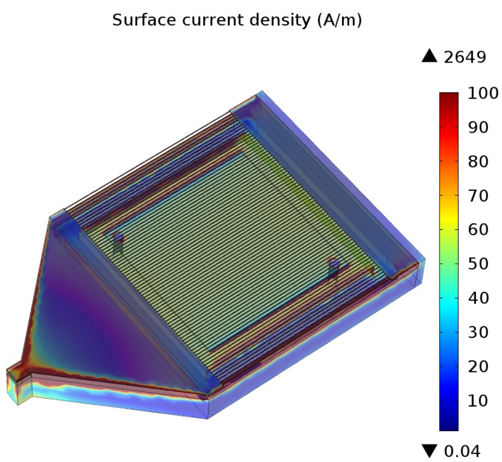

Figure 2: Surface current distribution on the surfaces of the coil

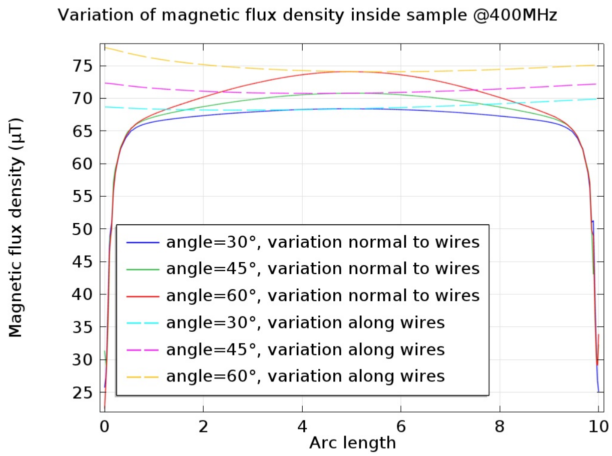

Figure 3: Magnetic flux density variation along characteristic lines in the sample region

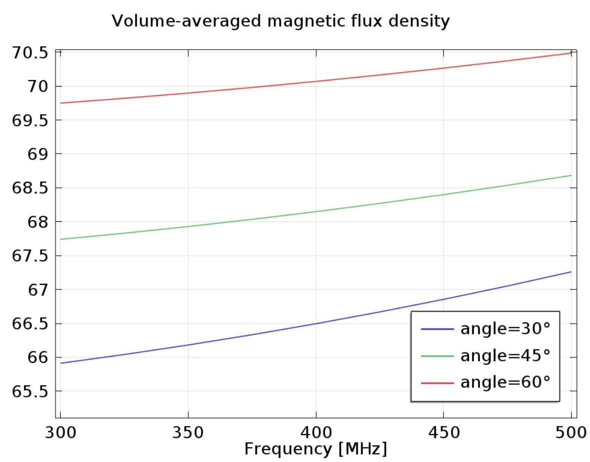

Figure 4: Volume-averaged magnetic flux density over the sample region