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Axially uniform magnetic field-modulation excitation for electron paramagnetic resonance in rectangular and cylindrical cavities by slot cutting

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ABSTRACT

In continuous-wave (CW) Electron Paramagnetic Resonance (EPR) a low-frequency time-harmonic magnetic field, called field modulation, is applied parallel to the static magnetic field and incident on the sample. Varying amplitude of the field modulation incident on the sample has consequences on spectral line-shape and line-height over the axis of the sample. Here we present a method of coupling magnetic field into the cavity using slots perpendicular to the sample axis where the slot depths are designed in such a way to produce an axially uniform magnetic field along the sample. Previous literature typically assumes a uniform cross-section and axial excitation due to the wavelength of the field modulation being much larger than the cavity. Through numerical analysis and insights obtained from the eigenfunction expansion of dyadic Green's functions, it is shown that evanescent standing-wave modes with complex cross-sections are formed within the cavity. From this analysis, a W-band (94 GHz) cylindrical cavity is designed where modulation slots are optimized to present a uniform 100 kHz field modulation over the length of the sample.

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1. Introduction

The problem described here has applications in continuous-wave (CW) Electron Paramagnetic Resonance (EPR) where low-frequency time-harmonic magnetic field, typically 100 kHz, is applied parallel to a static magnetic field incident on a microwave cavity. The low-frequency time-harmonic magnetic field, called field modulation, is coupled into the microwave cavity and modulates the resonance condition of the sample which offsets the EPR signal from the microwave carrier [1]. In order to maximize the field modulation incident on a sample the cavity can be designed in four ways: (i) the walls of the cavity are plated with silver that is electrically thin to the 100 kHz field modulation but at least 10 microwave skin-depths thick, (ii) design the cavity as a wire-wound structure, (iii) place the field-modulation coil inside of the cavity, or (iv) cut slots transverse to the cavity microwave current to break up field-modulation eddy-currents on the outside of the cavity.

Previous work from our laboratory focused on field-modulation eddy-current analysis of silver-plated graphite resonators and the effect of the wall thickness with respect to the fields incident on the sample [2]. Here, we focus on how cutting transverse slots into the side walls couples the incident field modulation into the cavity and the cross-sectional field-modulation profile that is formed. This method is used at high frequency EPR (above 94 GHz) where methods ii and iii become problematic [3,4] or when modulation frequencies are increased for use in Electron Nuclear Double Resonance (ENDOR) EPR spectroscopy [5]. An illustration of the scheme studied in this work is shown in Fig. 1, where the modulation coils are a Helmholtz pair in the *yz*-plane. This configuration is known as a Helmholtz pair. Although this method focuses on field modulation it is applicable to ENDOR frequencies if the cavity and coil is rotated by 90 degrees around the *z*-axis.

In general, the incident field modulation induces an electric field within the slots and evanescent modes are formed in the interior. To simplify the problem assume an infinitely long waveguide. EPR literature has not focused on the magnetic field cross-section of the induced field-modulation modes which has implications on sample line-shape, spin physics, and quantitative EPR [6]. Past and current literature assumes that the 100 kHz field modulation has such a large wavelength compared to the resonator body that it can be regarded as quasi-static. This work shows that complex cross-section standing-waves modes form in the cavity and

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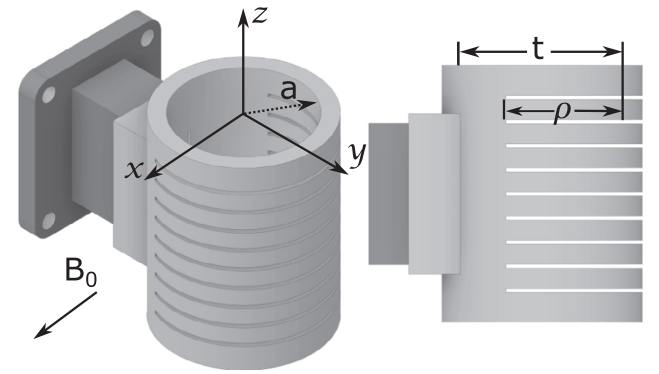

Fig. 1. A cylindrical TE_{011} cavity resonator (without end-sections) is shown with waveguide coupling, field-modulation slots, and coordinate system. The static magnetic field and applied field modulation are in the x-direction. The inner diameter is t, with radius a, and the slot depth is ρ.

propagate as evanescent modes along the z direction. These modes are formed from each slot and the interactions between slots. Understanding the coupling mechanism and field interactions gives insight into better EPR cavity design.

We present our results on two typical resonator geometries: a rectangular TE_{102} or cylindrical TE_{011} cavity. Here, the eigenfunction expansion for the dyadic Green's functions of magnetic types for rectangular and circular waveguides excited by a slot with an induced electric field induced by an externally homogeneous magnetic field are formulated. The eigenfunction expansion of $\overline{\overline{G}}_m$, known as the Ohm-Rayleigh method, is explicitly used to derive the dyadic Green's function of the magnetic field within the waveguide geometries [7,8]. The magnetic field solution for a single slot along the waveguide axis and a cross-sectional profile is presented. Multiple-slot geometry derivation is described using a simple summation (zero-order) of the individual slots and a method of moments (first-order) modification for slot-to-slot interactions. Ansys High Frequency Structure Simulator (HFSS; v. 17.0, Canonsburg, PA) is utilized to both validate and normalize the Green's function solutions. Good agreement is shown between Green's function and numerical data. The combined first-order method of moments dyadic Green's function solution for two slots gives insight on the interactions of multiple slots and yields phenomenological guidance in the design of EPR cavities.

From the insight gained, we describe a cylindrical cavity at W-band with modulation slots designed with varying depths which present a uniform 100 kHz field modulation on axis over the length of the sample. Additionally, the cylindrical cavity is a TE_{01U}, where the U subscript denotes that the microwave magnetic field is also uniform in the z-direction over the sample. It has been shown that the microwave magnetic field in a cavity can be made uniform by designing the cavity as a waveguide section at cut-off over the region of interest and proper end-sections to tune the cavity to the cut-off frequency [9–11]. This work presents the first uniform field-modulation and microwave magnetic field cavity resonator at W-band.

2. Methods

The dyadic Green's functions are derived using a number of references cited in this work and are solved by programming them into Wolfram (Champaign-Urbana, IL) Mathematica (version 10.0). Mathematica includes pre-defined parallel programming functions such as *ParallelSum* and *ParallelTable*. Using these functions, solutions to the dyadic Green's functions were accelerated by 76% resulting in solution times of approximately 2 min.

Parameters such as the electric field amplitude and profile within the slot are taken from Ansys HFSS solutions and used in the formulation of the dyadic Green's functions. This ensures that the dyadic Green's functions and HFSS solutions are directly comparable. Once all solutions are formed, the Green's function and numerical solutions are compared using both visual and analytical techniques. Visually, a two dimensional cross-section solution of the solved waveguide is plotted in a side-by-side comparison to view contour similarities.

Since this work focuses on an axial 100 kHz magnetic field, one must ensure the evanescent roll-off and field amplitude profile are properly reflected in the dyadic Green's function. A root-mean-square error (RMSE) function was employed to calculate the residual error between the normalized Green's function and numerical results. Using a RMSE is an accurate measurement to compare a calculated model (the dyadic Green's function) to the full-wave 3D simulation (Ansys HFSS) and has the unites of amps per meter (A/m). In order to calculate the RMSE both equations are discretized into n segments and directly compared according to

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{m=1}^{n}(H_{cal} - H_{sim})^2}[\mathrm{A/m}]. \tag{1}$$

where H_{cal} and H_{sim} are the magnetic field calculated by the dyadic Green's functions and the magnetic field simulated by Ansys HFSS, respectively. Both the visual and analytical analysis give confidence in the dyadic Green's function solutions to form a resulting insight and discussion of this work.

In order to minimize Mathematica calculation time, the number of modes that were solved in the analytical code was varied until the solutions had an acceptable convergence. It was found that using ten TE and nine TM evanescent modes resulted in more than adequate convergence. These results were consistent in rectangular and cylindrical waveguides.

3. Eigenfunction expansion of dyadic Green's functions

Time-harmonic electric and magnetic fields, $e^{-i\omega t}$, are assumed throughout the formulation of the problem and solutions.

3.1. Rectangular waveguide formulation

The rectangular waveguide is defined in Fig. 2, where $\hat{\mathbf{z}}$ is the propagation vector and the electromagnetic modes are bounded by $0 \leqslant x \leqslant a$ and $0 \leqslant y \leqslant b$. The vector wave equation is defined as

$$\nabla \times \nabla \times \overline{\Phi} - \kappa^2 \overline{\Phi} = 0, \tag{2}$$

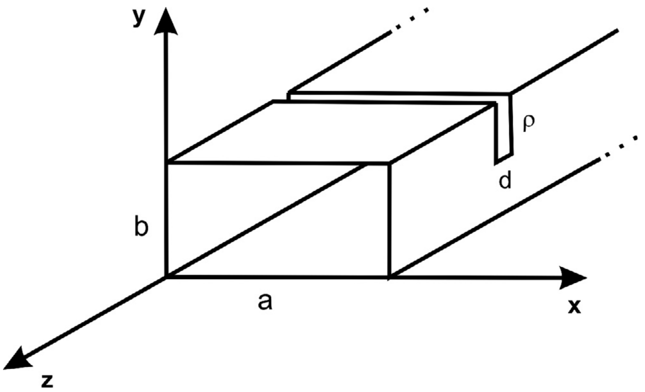

Fig. 2. Definition of the rectangular geometry with a slot thickness of d and a depth of ρ cut into the broad face of the waveguide. The walls of the waveguide are perfect electric conductor (PEC) material and have a cross-section of a by b. The waveguide wall thickness is not finite, but propagation is assumed instantaneous.

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