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# Analysis of two stacked cylindrical dielectric resonators in a $TE_{102}$ microwave cavity for magnetic resonance spectroscopy

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ABSTRACT

The frequency, field distributions and filling factors of a DR/$TE_{102}$ probe, consisting of two cylindrical dielectric resonators (DR1 and DR2) in a rectangular $TE_{102}$ cavity, are simulated and analyzed by finite element methods. The $TE^{+++}$ mode formed by the in-phase coupling of the $TE_{01\delta}$(DR1), $TE_{01\delta}$(DR2) and $TE_{102}$ basic modes, is the most appropriate mode for X-band EPR experiments. The corresponding simulated $B^{+++}$ fields of the $TE^{+++}$ mode have significant amplitudes at DR1, DR2 and the cavity's iris resulting in efficient coupling between the DR/$TE_{102}$ probe and the microwave bridge. At the experimental configuration, $B^{+++}$ in the vicinity of DR2 is much larger than that around DR1 indicating that DR1 mainly acts as a frequency tuner. In contrast to a simple microwave shield, the resonant cavity is an essential component of the probe that affects its frequency. The two dielectric resonators are always coupled and this is enhanced by the cavity. When DR1 and DR2 are close to the cavity walls, the $TE^{+++}$ frequency and $B^{+++}$ distribution are very similar to that of the empty $TE_{102}$ cavity. When all the experimental details are taken into account, the agreement between the experimental and simulated $TE^{+++}$ frequencies is excellent. This confirms that the resonating mode of the spectrometer's DR/$TE_{102}$ probe is the $TE^{+++}$ mode. Additional proof is obtained from $B_{1x}$, which is the calculated maximum x component of $B^{+++}$. It is predominantly due to DR2 and is approximately 4.4*G*. The $B_{1x}$ maximum value of the DR/$TE_{102}$ probe is found to be slightly larger than that for a single resonator in a cavity because DR1 further concentrates the cavity's magnetic field along its *x* axis. Even though DR1 slightly enhances the performance of the DR/$TE_{102}$ probe its main benefit is to act as a frequency tuner. A waveguide iris can be used to over-couple the DR/$TE_{102}$ probe and lower its *Q* to ≈150. Under these conditions, the probe has a short dead time and a large bandwidth. The DR/$TE_{102}$ probe's calculated conversion factor is approximately three times that of a regular cavity making it a good candidate for pulsed EPR experiments.



## 1. Introduction

Pulsed and continuous-wave (CW) electron resonance techniques, such as electron paramagnetic resonance (EPR) [1–6], electron–nuclear double resonance (ENDOR) [4,7–9], electron–electron double resonance (ELDOR) [4,6,10,11], electron spin echo envelope modulation (ESEEM) [9,12,13], double quantum coherence (DQC) [14–16] and double electron–electron resonance (DEER) [12,17–21], are powerful spectroscopic methods for studying the magneto-structural properties of molecules containing unpaired electrons. They are becoming the experimental methods of choice to determine spin–spin distances, geometry, structures and gyromagnetic, fine, and hyperfine tensors of paramagnetic molecules of biological and medicinal significance. The paramagnetic centers in these large biological molecules are usually dilute and the sample size is mostly small and limited. Consequently, considerable research is spent on increasing spectrometer sensitivity to facilitate their detection.

One of the ways to increase a spectrometer's sensitivity and signal-to-noise ratio (SNR) is by substituting its resonant cavities by miniature loop-gap (LGR) [22–28] and dielectric (DR) resonators [29–41]. These resonators have several advantages over metal-walled cavities such as small size, low cost, high energy density in the sample vicinity, large magnetic fields ($B_1$) and filling factors [22–36].

The use of loop-gap resonators is more widespread than DRs and they are now commonly used in EPR spectrometers. They have been reviewed, on more than one occasion, by Hyde et al. [42,43].

As early as 1964 Rosenbaum [29], followed by Walsh and Rupp [37], were the first to employ a DR instead of a cavity in an EPR spectrometer. While DRs have comparable performance to LGRs, some have background signals due to paramagnetic impurities [40]. These may become apparent at low temperatures. Their contribution to the overall spectra is eliminated by subtracting the spectrum of the empty resonator from that containing the sample.

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The coupling and tuning of a LGR or DR to an EPR spectrometer's microwave bridge is not an easy task [44]. A theoretical account of this subject has recently been given by Mett et al. [45]. For LGRs and DRs coupling is typically carried out by means of a wire loop of appropriate diameter and critical coupling is achieved by varying the distance between the resonator and the loop [22,24,30,35,46]. Waveguide irises [25], Gordon couplers [47] and other antennae [48] have also been used to critically couple LGRs to the spectrometer's microwave bridge.

Usually a shield is used to house LGRs and confine the microwave radiation. Dielectric resonators have been housed in microwave shields as well [32–36]. For example, DRs placed a microwave shield have been used for high pressure [30], stopped flow and rapid scan [33] EPR. The theory of doubly stacked resonators in a microwave shield has been discussed by Jaworski et al. [32].

In addition to the convenient coupling via a waveguide iris, cavities serve the same purpose as a microwave shield and have also been used to house LGRs [49,50] and DRs. A *single* resonator placed in a $TE_{102}$ cavity was studied by different groups [31,38,40,41]. Nesmalov et al. studied a single ferroelectric resonator in a $TM_{110}$ Cavity [40], while and Golovina et al. employed a cylindrical $TE_{011}$ cavity [38].

The DR/$TE_{102}$ probe used in our laboratory consists of a pair of dielectric resonators, with $\varepsilon_r = 29.2$, in an unmodified $TE_{102}$ rectangular cavity. Thus a regular EPR cavity is converted into a dielectric probe with higher SNRs that are at least 24 times larger than the $TE_{102}$ cavity alone [39]. In addition, the frequency of the resonator can be tuned over an extended range. The frequency of the DR/$TE_{102}$ probe is coarsely tuned by varying the distance between the two dielectric resonators. Once the appropriate frequency range is determined, it is then *fine* tuned by keeping that distance constant and changing resonators' positions along the cavity $x$ axis where the sample tube resides. As a result, the two dielectric resonators are asymmetrically positioned in the $TE_{102}$ cavity.

In this article one attempts to numerically assess by simulation [51], using the finite integration methods [52], the microwave electric and magnetic field distributions, sensitivity, filling factors and frequency behavior of the DR/$TE_{102}$ probe used in our EPR spectrometers.

The paper is partitioned as follows. In Section 1 the problem and the goals of the work are presented. Section 2 provides a theoretical background on the linear combination of the electromagnetic fields for two dielectric resonators in a rectangular cavity. In Section 3 a description of the numerical and experimental methods is given while Section 4 is divided into three subsections that present and discuss the results. The first subsection deals with the properties of two identical dielectric resonators symmetrically placed in a $TE_{102}$ cavity while the next section discusses the results of positioning them asymmetrically in the cavity. Section 4.3 compares the magnetic field distributions of one and two resonators in a $TE_{102}$ cavity. Section 5 summarizes the results and conclusions of the work.

## 2. Theoretical background

In the previous analyses of an EPR probe formed by stacking two dielectric resonators the shield was not considered to be a resonator with distinct resonant modes but simply imposed boundary conditions due to its electrical conducting walls [32,53]. Mett et al. were the first to simulate the effect of a cylindrical cavity as a resonating entity on a single dielectric resonator [54].

In general, two dielectric resonators, DR1 and DR2, in a conducting cavity can be regarded as a combined system of three coupled structures. Consequently, the coupling of any three basic modes arising from DR1, DR2 and the cavity results in three new modes that are approximated as a linear combination of the basic ones. These new coupled modes will differ from one another according to the relative phases and coupling coefficients of their basic modes. Here, the individual DR1, DR2 and cavity basic modes are $TE_{01\delta}$, $TE_{01\delta}$ and $TE_{102}$ respectively. They give rise to the three coupled modes, $TE^{+++}$, $TE^{++-}$ and $TE^{+--}$.

Their corresponding spatial electric and magnetic field components, **E** and **B**, are

$$\mathbf{E}^{+++} = a_1^{+++}\mathbf{E}_{01\delta}(\mathrm{DR1}) + a_2^{+++}\mathbf{E}_{01\delta}(\mathrm{DR2}) + a_3^{+++}\mathbf{E}_{102}, \tag{1}$$

$$\mathbf{E}^{++-} = a_1^{++-}\mathbf{E}_{01\delta}(\mathrm{DR1}) + a_2^{++-}\mathbf{E}_{01\delta}(\mathrm{DR2}) - a_3^{++-}\mathbf{E}_{102}, \tag{2}$$

$$\mathbf{E}^{+--} = a_1^{+--}\mathbf{E}_{01\delta}(\mathrm{DR1}) - a_2^{+--}\mathbf{E}_{01\delta}(\mathrm{DR2}) - a_3^{+--}\mathbf{E}_{102}, \tag{3}$$

$$\mathbf{B}^{+++} = b_1^{+++}\mathbf{B}_{01\delta}(\mathrm{DR1}) + b_2^{+++}\mathbf{B}_{01\delta}(\mathrm{DR2}) + b_3^{+++}\mathbf{B}_{102}, \tag{4}$$

$$\mathbf{B}^{++-} = b_1^{++-}\mathbf{B}_{01\delta}(\mathrm{DR1}) + b_2^{++-}\mathbf{B}_{01\delta}(\mathrm{DR2}) - b_2^{++-}\mathbf{B}_{102}, \tag{5}$$

and

$$\mathbf{B}^{+--} = b_1^{+--}\mathbf{B}_{01\delta}(\mathrm{DR1}) - b_2^{+--}\mathbf{B}_{01\delta}(\mathrm{DR2}) - b_3^{+--}\mathbf{B}_{102}. \tag{6}$$

Here $a_i^{\pm\pm\pm}$ and $b_i^{\pm\pm\pm}$ are the coupling coefficients where the ±superscripts indicate the relative phase between the modes, which can be either 0° or 180°. The frequency, composition and electromagnetic fields of the new modes will depend on their dimensions and relative positions. As an example, the simulated magnetic field modes, $\mathbf{B}^{+++}$, $\mathbf{B}^{++-}$ and $\mathbf{B}^{+--}$, are schematically drawn in Fig. 1a–c.

The comparison of Fig. 1a–c shows that the modes in Fig. 1a and b have a larger $TE_{102}$ component than that in Fig. 1c. The small $TE_{102}$ component of $TE^{+--}$, causes its $\mathbf{B}^{+--}$ fields, shown in Fig. 1c, to be very small near the cavity walls. Therefore this mode is not suitable for the exciting the DR1 and DR2 resonators via the cavity iris.

The further comparison of Fig. 1a and b in the vicinity of DR1 and DR2 shows that $\mathbf{B}^{+++}$ is larger than $\mathbf{B}^{++-}$.

Consequently, using the $TE^{+++}$ mode should result in a spectrometer with a relatively higher SNR and sensitivity.

In general, linear combinations of other $TE_{mnp}$, $TM_{mnp}$ and hybrid modes may also exist. For example the DR1 and DR2 $TE_{01\delta}$ modes may form linear combinations with the cavity's $TE_{101}$ mode, as will be shown later.

## 3. Computational and experimental details

A computer employing two Quad-Core Opteron 2350 Processors, with 3 GB of RAM and running Windows XP was used for the simulations. The DR/$TE_{102}$ properties were calculated using the Computer Simulation Technology (CST), suite of programs [51]. The dimensions, relative positions in space and dielectric constants of DR1, DR2 and cavity are used as inputs. The program solves Maxwell's equations, using an eigenvalue formalism, from which the frequencies, filling factors, electric and magnetic field distributions are calculated. The program can use two methods for solving the eigenvalue problem. The first is the Jacobi–Davidson (JD) method [55], while the second is the Advanced Krylov Subspace (AKS) method [56]. The JD method is computationally expensive and time consuming but is robust when solving degenerate modes. Since, due to its low symmetry, the system under consideration has no degeneracies, the faster AKS method was used. During the solution, the system's geometry is spatially partitioned into a mesh of grid elements. The equations are then solved using these grid elements by the finite integration technique (FIT) [52].

The EPR spectrum of the $Mn^{2+}$/CaO sample, used as a reference standard, was recorded with a modified Varian E104 spectrometer [39]. The frequency of the DR/$TE_{102}$ resonator was measured with a Hewlet-Packard model HP5340A frequency counter and the