Accurate Analysis of Whispering Gallery Modes in Dielectric Resonators with BoR FDTD Method

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Abstract—This paper presents an accurate approach to FDTD analysis of whispering gallery modes in dielectric resonators. In those problems resonant frequencies are supposed to be extracted with relative errors below 10^{-4}. It is widely believed that only custom-made software codes, based on mode matching methods, can meet such stringent accuracy requirements. Herein, we demonstrate how the required accuracy can be obtained with a general-purpose FDTD code, run within a new three-step procedure. Advantages of the FDTD approach include more flexibility in modelling scenarios with unusual shapes or/and lossy materials.

Keywords—Dielectric resonators, whispering gallery modes, EM simulations, FDTD method, bodies of revolution.

I. INTRODUCTION

In a classical paper [1] the authors investigate a cooled dielectric resonator composed of a flat sapphire ring with a supporting rod fixing it in a metal box (Fig. 1). They provide an excellent comparative material composed of very precise measurements with micrometre tolerances of object dimensions and resonant frequency measurements of 10^{-6} accuracy.

Application of such dielectric resonators for accurate material measurements at microwave frequencies (around 10 GHz in [1]) requires that the measured resonances be reproduced within 1 MHz (or 10^{-4}) in computer modelling. The authors of [1] apply a custom-made code that hybridises radial mode-matching and Rayleigh-Ritz techniques. For only 4 out of 22 considered whispering-gallery modes, the computed results differ from the measured ones by more than 1 MHz (with maximum error close to 3 MHz). However, a limitation of the applied numerical technique is that it would need re-programming for different structure shapes.

On the other hand, many general-purpose electromagnetic (EM) simulators appeared on the market since the publication [1], many of them based on the Finite Difference Time Domain (FDTD) scheme. The authors of the present paper have had many discussions with researchers in the field, who tried to use FDTD as a retro-modelling tool for dielectric measurements. Their typical conclusion was: it was impossible and 10^{-4} accuracy could not be reached.

Herein, we demonstrate that the Body of Revolution (BoR) version of FDTD, as described in e.g. [2] and implemented in commercial software [3], does provide the required accuracy when run within a specific procedure. Our findings show that accurate computations as in [1] are accessible with general-purpose codes, without any need for customised programming. Moreover, new horizons open up for application of a wider class of resonators and samples, including those with irregular (though axisymmetrical) shapes and/or lossy metal parts.

II. THE SIMULATION PROCEDURE

In BoR FDTD the modelled scenario is reduced to two dimensions (2D) as in Fig. 2. Angular dependence of the fields is imposed analytically [2]. In Fig. 2, the axis of symmetry is shown at the bottom of the simulation domain and the radial direction is upwards. There is also a vertical symmetry plane, which enters into simulation as an electric wall for N-modes or as a magnetic wall for S-modes, as defined in [1]. Thus we consider one layer of FDTD cells distributed over a quarter of the longitudinal section of the resonator. Meshing shown in Fig. 2 corresponds to FDTD cell size of 0.2 mm in sapphire, relaxed to 0.5 mm in air. According to 3D FDTD dispersion analysis [4], the resulting ca. 50 cells per wavelength in sapphire should suppress numerical errors to 0.05%.

Our simulation procedure is composed of three steps:


A. Investigating possible modes using QProny method.

A virtual lumped source of finite internal impedance and a soft probe are applied to selected field components (in, out in Fig. 2). The scenario is excited by a Gaussian pulse covering the spectrum of interest (here [1], 8 GHz to 12 GHz). We modify the position, orientation, and impedance of the source to induce desired modes and to control coupling. Signal postprocessing with Generalised Pencil of Function (GPOF) method [5] implemented in the QProny module [3] detects the existing modes and their Q-factors.

Computation of this step completes within 1 minute. However, performance of the applied GPOF is known to deteriorate for waveform sampling at over 256 points per period [5]. Indeed, in the considered extremely finely meshed example we have not been able to obtain results converged better than $3 \times 10^{-4}$ accuracy. We have then run step B.

B. Accuracy refinement for selected modes.

We repeat a BoR FDTD simulation using a Gaussian pulse of a narrow spectrum around one of the resonances detected in point A. Direct Fourier Transform is applied to signals at the source and probe. While such a procedure may require quite a large number of FDTD iterations (ca. 600 000), it proceeds fast since the circuit has a small number of cells (ca. 16 000) and a standard laptop computer executes 1 500-2 000 iterations per second. One complete FDTD analysis takes 5-10 minutes.

C. Investigating field distribution of particular modes.

Once the resonant frequency is known, we can excite the scenario with a sinusoidal waveform. With functionalities as in [3] we visualise 3D patterns of fields and dissipated power.

<table>
<thead>
<tr>
<th>Mode - ang. var.</th>
<th>$f_1$ [MHz]</th>
<th>$f$ [MHz]</th>
<th>$\Delta f$ [MHz]</th>
<th>relative error $10^6 \Delta f / f_1$</th>
<th>$f_c$ [MHz]</th>
</tr>
</thead>
<tbody>
<tr>
<td>N4 - 8</td>
<td>8512.81</td>
<td>8512.86</td>
<td>+ 0.05</td>
<td>0.06</td>
<td>8513.17</td>
</tr>
<tr>
<td>N4 - 9</td>
<td>9191.15</td>
<td>9191.22</td>
<td>+ 0.07</td>
<td>0.07</td>
<td>9191.34</td>
</tr>
<tr>
<td>N4 - 10</td>
<td>9864.02</td>
<td>9864.10</td>
<td>+ 0.08</td>
<td>0.08</td>
<td>9864.08</td>
</tr>
<tr>
<td>N4 - 11</td>
<td>10531.88</td>
<td>10531.90</td>
<td>+ 0.02</td>
<td>0.02</td>
<td>10529.60</td>
</tr>
<tr>
<td>N4 - 13</td>
<td>11855.00</td>
<td>11854.38</td>
<td>- 0.62</td>
<td>0.52</td>
<td>11852.06</td>
</tr>
<tr>
<td>S1 - 10</td>
<td>8217.60</td>
<td>8217.51</td>
<td>- 0.09</td>
<td>0.11</td>
<td>8218.69</td>
</tr>
<tr>
<td>S1 - 11</td>
<td>8805.50</td>
<td>8805.26</td>
<td>- 0.26</td>
<td>0.29</td>
<td>8806.33</td>
</tr>
<tr>
<td>S1 - 12</td>
<td>9395.86</td>
<td>9395.08</td>
<td>- 0.68</td>
<td>0.63</td>
<td>9396.12</td>
</tr>
<tr>
<td>S1 - 13</td>
<td>9987.20</td>
<td>9886.42</td>
<td>- 0.78</td>
<td>0.78</td>
<td>9987.64</td>
</tr>
<tr>
<td>S1 - 14</td>
<td>10580.00</td>
<td>10579.33</td>
<td>- 0.67</td>
<td>0.63</td>
<td>10580.31</td>
</tr>
<tr>
<td>S1 - 15</td>
<td>11173.80</td>
<td>11173.05</td>
<td>- 0.64</td>
<td>0.57</td>
<td>11173.89</td>
</tr>
</tbody>
</table>

III. SIMULATION RESULTS AND DISCUSSION

The proposed BoR FDTD procedure has been applied to extract resonant frequencies of 11 whispering - gallery modes in the sapphire resonator after [1]. Our results are summarised and compared to the data of [1] in Table I. A maximum deviation of BoR FDTD from the measurements of [1] is 0.78 MHz. This satisfies the requirement of absolute 1 MHz (and relative $10^6$) accuracy for practical applications of dielectric resonators in microwave material measurements [1].

The BoR FDTD algorithm run on a contemporary laptop has neared the performance previously unique to problem-tailored algorithms. Additionally, it offers more flexibility than e.g. radial mode - matching as in [1], in direct modelling of real (lossy) metal enclosures and more general (non - cylindrical) axisymmetrical samples.

We have observed that relative errors of resonant frequency extraction ($<0.008\%$) are less than expected based on classical 3D FDTD error bounds (ca. 0.05\%), especially for the N-modes. Intuitively, we attribute this to the fact that the fields vary quickly in the angular direction, which is modelled analytically, but slowly in the 2D plane, where the finite - difference approximation is applied. However, rigorous estimation of error bounds for BoR FDTD is needed to better understand its convergence and prudently control its 2D mesh.

Further work will be conducted in the following directions:

1. Development of GPOF method after [5] for accurately postprocessing signals oversampled at more than 256 points per period. This will accelerate the extraction of resonant frequencies by curtailing step B of the procedure.

2. Application of BoR FDTD to evaluate the effects of imperfect cylindricity of practically manufactured samples (non - flat top and bottom surfaces, conical side walls or chamfered edges) and metal losses on the results of complex permittivity measurements.

3. Rigorous derivation of error bounds for BoR FDTD, following the characteristic equation approach previously developed in Cartesian coordinates [4] and taking into account dielectrics [6]. This will facilitate mesh optimisation for desired accuracy.

Extended results will be presented at the conference.

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REFERENCES


