Accurate determination of the quality factor of axisymmetric resonators by use of a perfectly matched layer

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Abstract

Numerical methods are required to develop an accurate electromagnetic model for various axisymmetric resonators such as micro-discs and micro-toroids. A finite element model for such resonators already exists, however there are number of issues with that model: 1) No perfectly matched layer or any other absorbing boundary conditions are used, 2) Quality factor of a micro-cavity is estimated by running the model multiple times with different boundary conditions, 3) Prior knowledge of the mode frequency is required to implement one of the boundary conditions, and 4) Quality factor of only one mode is estimated at a time. Here our purpose is to overcome these drawbacks and determine the quality factor of axisymmetric resonators with high accuracy by using the perfectly matched layer in a finite element model.

1 Introduction

Perfectly matched layers (PML) act as artificial boundaries that truncate the computation domain of open region scattering problems in the finite element method. The whispering gallery modes (WGM) of an open micro-cavity radiate into the surroundings and a PML is required in order to block the unwanted reflections from the boundaries of the computation domain. There have been previous attempts of developing finite element models (FEM) of axisymmetric cavities along with the PML. In 2005, Chinellato et al. [1] showed a FEM model which was implemented in MATLAB. However, their model failed to simulate the resonators with large size. In their work they solved the numerical examples of dielectric spheres of sizes less than $3\mu m$. In 2009, Karl et al. developed a FEM model for studying a micro-pillar cavity [2]. But in their model they did not consider the suppression of false solutions, a well known problem in finite element formulations [3]. Moreover, they estimated the quality factor of the modes by fitting the Lorentzian peak to the calculated spectrum of the cavity, thus an extra approximation had been introduced.

In 2007, Oxborrow [4] developed a FEM for open axisymmetric resonators in COMSOL. In his work, he showed that the model could simulate an arbitrary cross section resonators in optical and microwave regimes, thus removing the size limitation in [1]. Another difference from [1] is in terms of suppression of false modes; Oxborrow used a simple penalty term in his master equation whereas Chinellato et al. used Nédélec edge and modified Lagrange nodal element functions to avoid the spurious modes. However in Oxborrow’s model no PML was implemented and as a result the WGM quality factor could not be determined accurately. The quality factor due to the WGM radiation was estimated by placing a bound on its minimum and maximum possible values. These maximum and minimum values were determined by executing the model multiple times with different boundary conditions. Moreover, the model lacks the capability to estimate the quality factor of multiple modes simultaneously.

Determination of the quality factor with high accuracy is important in certain applications such as cavity ring down spectroscopy where decay time depends upon the quality
factor. In order to provide accurate determination of the WGM quality factor, we have improved Oxborrow’s model by modifying its master equation and implementing the PML along the boundaries of the computation domain. The modified model does not have any of the drawbacks of the previous model. Moreover, we have computed the quality factors of all the modes without using any fitting algorithms.

In our model, we treat the PML as an anisotropic absorber and implement it in the cylindrical coordinate system. Our model is applicable to any axisymmetric resonator geometry but due to the availability of analytical expressions for spherical resonators, we have tested the model by determining the quality factors of a silica micro-sphere in air. We have found that our simulation results are in excellent agreement with the analytical results. We also apply our model to micro-toroids and show that our results are consistent with those obtained by experiment. By using PML, our model has also overcome all discrepancies present in the previous models.

2 Mathematical Description

Applying Galerkin’s method to the wave equation and after using the boundary conditions for open resonators, one can arrive at the FEM equation in the weak form [4]:

$$
\int_V \left( \nabla \times \vec{H}^* \right) \epsilon^{-1} \left( \nabla \times \vec{H} \right) - \alpha (\nabla \cdot \vec{H}^*) (\nabla \cdot \vec{H}) + c^{-2} \vec{H}^* \cdot \partial^2 \vec{H} \over \partial t^2 \right) dV
$$

(1)

where \( \vec{H} \) represents the magnetic field of the resonator and \( \vec{H}^* \) represents the test magnetic field, an essential component of the weak form. The second term of the equation 1 represents a penalty term to suppress false solutions. None of the field components will depend upon the azimuthal coordinate \( \phi \) in the axisymmetric resonators, resulting in reduction of the 3D problem to a 2D problem.

2.1 PML Formulation

A PML can be treated as an anisotropic absorber in which the diagonal permittivity and permeability tensors of the absorber are modified according to equation 2 [5].

$$
\bar{\epsilon} = \epsilon \tilde{\Lambda}, \bar{\mu} = \mu \tilde{\Lambda},
$$

(2)

The radial and axial modification factors are represented by \( \tilde{\Lambda} \), which is given by equation 3

$$
\tilde{\Lambda} = \left( \begin{array}{c} \tilde{s}_r \\ \tilde{s}_z \end{array} \right) = \left( \begin{array}{c} \frac{\tilde{r}}{\tilde{r}} \\ \frac{\tilde{z}}{\tilde{z}} \end{array} \right) = \left( \begin{array}{c} \tilde{s}_r \\ \tilde{s}_z \end{array} \right) \tilde{\Lambda} + \left( \begin{array}{c} \tilde{s}_r \\ \tilde{s}_z \end{array} \right) \frac{\partial}{\partial \tilde{r}} + \left( \begin{array}{c} \tilde{s}_r \\ \tilde{s}_z \end{array} \right) \frac{\partial}{\partial \tilde{z}}
$$

(3)

where

$$
\tilde{s}_r = \begin{cases} n_{\text{medium}} \\ n_{\text{medium}} - jG \left( \frac{r - r_{\text{pml}}}{t_{\text{pml}}} \right)^N \end{cases} \begin{cases} 0 \leq r \leq r_{\text{pml}} \\ r > r_{\text{pml}} \end{cases}
$$

$$
\tilde{s}_z = \begin{cases} n_{\text{medium}} \\ n_{\text{medium}} - jG \left( \frac{z - z_{\text{pml}}}{t_{\text{pml}}} \right)^N \end{cases} \begin{cases} 0 \leq z \leq z_{\text{pml}} \\ z > z_{\text{pml}} \end{cases}
$$

$$
\tilde{r} = \begin{cases} \frac{r}{r - jG} \left( \frac{r - r_{\text{pml}}}{r_{\text{pml}}} \right)^N + 1 \ \ \ (N + 1)^t_{\text{pml}} \end{cases} \begin{cases} 0 \leq r \leq r_{\text{pml}} \\ r > r_{\text{pml}} \end{cases}
$$
where \( t_{rpml}, t_{upml}, t_{lpml} \) are the PML thicknesses in the radial, +z and -z directions respectively and \( r_{pml}, z_{upml}, z_{lpml} \) are the locations of the start of PML in the radial, +z and -z directions respectively. \( n_{medium} \) is refractive index of the medium, \( N \) is order of the PML, and \( G \) is a positive integer.

In the PML expressions \((s_r, s_z, \tilde{r})\), the imaginary component contributes to the attenuation of waves in the PML but at the same time, due to the discrete nature of the FEM mesh, a large imaginary component will introduce reflections at the interface between the PML and the medium. In order to determine the optimal value for the imaginary component, we have investigated linear, quadratic, and cubic PML of different thicknesses for various values of \( G \) by running many simulations for various sphere diameters. To deduce the optimum values of the parameters, we then compared the simulation results for \( Q_{WGM} \) of spherical cavities with the analytical ones [10]. The simulation results show that a linear (i.e. \( N = 1 \)), and \( \lambda/4 \) thick PML with a \( G \) value of 5 is optimum. We have also used these optimum values for the simulations of the disc and the toroidal cavities.

2.2 FEM equation with PML

In order to incorporate the PML, we have reformulated equation 1 in the following way:

\[
\int_{V} \left( (\nabla \times \vec{H}) \epsilon^{-1}(\nabla \times \tilde{H}) - \alpha(\nabla \cdot \vec{H}) (\nabla \cdot \tilde{H}) + c^{-2} \vec{H} \cdot \hat{\mu} \cdot \frac{\partial^2 \vec{H}}{\partial t^2} \right) dV
\]  

(4)

By casting equation 4 into the FEM software COMSOL, a full vectorial finite element model of a silica sphere in air can be obtained. By using the eigenvalue solver in COMSOL, resonant frequencies of all the modes can easily be determined. Since the PML introduces losses in the computational domain, the resonant frequency \((f_r)\) will be a complex number and the quality factor due to the WGM radiation can be calculated as:

\[
Q_{wgm} = \frac{\Re(f_r)}{2\Im(f_r)}
\]  

(5)

2.3 Analytical expressions of the spherical resonator

The quality factor due to WGM radiation losses in a spherical micro-cavity can be written as [6]:

\[
Q_{wgm} = \frac{1}{2}(m + 1)^{p^{1-2M}(p^2 - 1)^{\frac{1}{2}}} e^{2T_m}, \quad m \gg 1
\]  

(6)

where

\[
m = \text{azimuthal mode number}
\]

\[
p^2 = \frac{\epsilon_{\text{sphere}}}{\epsilon_{\text{medium}}}
\]

\[
T_m = (m + 1)^2 (m - \tanh(m))
\]

\[
m_l = \cosh^{-1} \left( \frac{1}{m + \frac{1}{2}} \left( q^{\beta} + \frac{p^{1-2M}}{\sqrt{(p^2 - 1)}} \right)^{-1} \right)
\]

\[
\beta = \left( \frac{1}{2} \left( m + \frac{1}{2} \right) \right)^{\frac{1}{2}}
\]

\[
M = \begin{cases} 
0 & \text{For TE} \\
1 & \text{For TM} 
\end{cases}
\]
\( q^{th} \) root of equation \( F_{\text{airy}}(t^q) = 0 \)

\[ m \text{ can be calculated using the characteristic equation for WGM frequencies } [7]: \]

\[ p^{1-2M} \frac{j_m(pk_0a)}{j_m(pk_0a)} = \frac{h^{'m}[k_0a]}{h_m[k_0a]} \]

where \( j \), \( h \) are Bessel functions, \( k_0 \) is the wave number \((2\pi/\lambda_0)\), and \( a \) is the radius of a microsphere.

It should be noted that equation 6 is an asymptotic solution for the Q\(_{\text{wgm}}\) of the spherical resonator which requires \( m \gg 1 \), however the error is less than 1% for \( m \geq 19 \) [9]. In our comparison for the analytical results, we have applied equation 6 to silica spheres with mode numbers (m) ranging from 27 – 98.

3 Results

Fig. 1 shows the TE and TM fundamental modes of a silica spherical cavity in air. We have plotted the quality factor due to the TE/TM fundamental whispering gallery mode radiation for various sphere diameters at 850nm. Fig. 2 shows the comparison of the FEM simulation results and results obtained by using analytical expressions presented in section 2.3. We have also calculated the minimum and maximum \( Q_{\text{wgm}} \) values using Oxborrow’s model [4] for each sphere diameter and those are also shown in Fig. 2.

From the simulation results, it is clear that the analytical results confirm the accuracy of our finite element model. The quality factors for all the modes (TE, TM fields of the fundamental and higher order modes) are also obtained by one single simulation rather than multiple simulations. Moreover, no prior knowledge of any of the mode frequencies is required to obtain the quality factors.

4 Discussion and application to other axisymmetric resonator geometries

The excellent agreement between the simulation and analytical results shows that the PML is absorbing the radiated waves effectively. However, the simulation results indicate that there are less reflections from the PML for the TM modes and values of quality factors for the TM modes are more accurate than the TE modes. This suggests that the PML is absorbing TM waves better than the TE waves. One possible explanation is that since the TM component is parallel to the radial PML so it will remain continuous along its boundary which will result in reflections only due to the discretization of the computation domain.

Our PML model is appropriate for other axisymmetric resonators where analytical solutions are not available. In order to test this, we have applied the FEM model to micro-toroid and micro-disc resonators, employing the same PML parameter values that were determined in section 2.1.

Armani et. al [8] demonstrated toroidal micro-cavities \((160 - 240 \mu m \text{ diameter and } 5 - 10 \mu m \text{ toroid thickness})\) which can exhibit quality factors in excess of \(10^8\). We tested our model for toroidal micro-cavities of the same geometry and found that the overall quality factor was also greater than \(10^8\).

Oxborrow [4] estimated the \( Q_{\text{wgm}} \) in the range of \(1.31 - 3.82 \times 10^7\) of a certain micro-disc resonator. We also calculated the \( Q_{\text{wgm}} \) of the same micro-disc and found the value of \(7.98 \times 10^6\) which lies within an order of magnitude of Oxborrow’s estimate. We believe that our value is a better estimate as Oxborrow’s upper and lower bounds are also less accurate for the micro-spheres (Fig. 2). In addition, our finite element model, without any approximation in its master equation and coupled with a PML, does not only give accurate quality factors,
Figure 1: False color surface plot of logarithmic intensity of magnetic field of the fundamental mode of a 12\(\mu m\) silica micro-sphere in air.
Figure 2: WGM Quality factors for various silica sphere diameters, upper and lower bounds correspond to the values calculated by using Oxborrow’s model [4].
but also determines the important parameters accurately for wide range of applications based on the axisymmetric micro-cavities such as biosensing, non-linear processes, and lasers.

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References

[1] O. Chinellato, P. Arbenz, M. Streiff, and A. Witzig, “Computation of optical modes in axisymmetric open cavity resonators,” Future Generation Computer Systems, 21, 1263–1274 (2005).

[2] M. Karl, B. Kettner, S. Burger, F. Schmidt, H. Kalt, and M. Hetterich, “Dependencies of micro-pillar cavity quality factors calculated with finite element methods,” Optics Express, 2, (2009).

[3] RA Osegueda, JH Pierluissi, LM Gil, A Revilla, GJ Villalva, GJ Dick, DG Santiago, and RT Wang, “Azimuthally dependent finite element solution to the cylindrical resonator,” 10th annual review of progress in applied computational electromagnetics, 1, 159–170, (1994).

[4] Mark Oxborrow, “Traceable 2-D finite element simulation of the whispering gallery modes of axisymmetric electromagnetic resonators,” IEEE Transactions on Microwave Theory and Techniques, 55, 1209–1218 (2007).

[5] J Jin, The finite element method in electromagnetics, John Wiley, USA, 2002, pp. 375-390.

[6] V. V. Datsyuk, “Some characteristics of resonant electromagnetic modes in a dielectric sphere,” Applied Physics, B54, 184–187, (1992).

[7] Lev Albertovich Weinstein, Open Resonators and Open Waveguides, The Golem Press, Boulder, Colorado, USA, 1969, pp. 298.

[8] D. K. Armani, T. J. Kippenberg, S. M. Spillane, and K. J. Vahala, “Ultra-high-Q toroid microcavity on a chip,” Nature, 421, 925–928 (2003).

[9] J. R. Buck, and H. J. Kimble, “Optimal sizes of dielectric microspheres for cavity QED with strong coupling,” Physical Review A, 67 033806 (2003).

[10] COMSOL code for the simulations is present at http://www.ece.mcgill.ca/~mcheem2/cheema_res.html.