Accurate Study of Q-Factor of Resonator by a Finite-Difference Time-Domain Method

Chi Wang, Ben-Qing Gao, and Ci-Ping Deng

***Abstract*—This paper describes the application of the finite-difference time-domain method to find the resonators' Q-factors. There are some techniques which can be used to reach it. One way is to directly compute the power loss using the surface impedance boundary condition (SIBC). The other is to incorporate the perturbation techniques to calculate the Q-value. The rectangular and cylindrical cavities have been studied by these method. A number of super conductor-sapphire microwave resonators with extra high Q-values have been studied. The results are very good in accuracy.**

I. Introduction

Q-FACTOR is an important parameter that indicates the property of the resonators. The study of the compact microwave resonators composed of the new materials with different conductivity needs an efficient method to compute the Q-factor of the resonator. But it is usually difficult to obtain the Q-factor, especially when the structure of the resonator is complex, for its exact EM field solution is quite complicated.

The finite-difference time-domain (FDTD) method, first proposed by Yee [1], permits one to study the electromagnetic waves with objects of arbitrary shape and material composition. It has been used for a wide variety of applications including scattering, absorption, bioelectromagnetics and antennas. Recently it has been applied to determine the resonant frequencies of the resonators [2]–[4]. However, there has been few applications of the method to the Q-factor of the resonator.

In this paper we present two ways to apply the finite-difference time-domain (FDTD) method, and with the help of the discrete Fourier transform to obtain the Q-factor of the resonators. One is based on the surface impedance boundary condition (SIBC) techniques [7]–[10] by direct computing the power loss between periods, which can study most of the practical resonators and it is especially suitable to study low-Q resonators; the other is based on the perturbation method which is very efficient and convenient to solve high Q and extra-high Q value problems.

In Section II, the numerical methods are described, and in Section III the numerical results are compared with theoretical solutions. A kind of high Tc super-conductor-sapphire microwave resonator with extremely high Q-value [13] is also studied, the numerical results are compared with the experimental results and the results in [13].

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II. Description of the Method

The computation of the resonator's Q value requires the EM field distribution first, which can be achieved by FDTD method.

The excitation pulse used in this work is chosen to be the square shape which has abundant frequency components so that the many modes can be excited. After the initial field is injected, the electromagnetic fields are established in the resonator. The fields not belonging to resonant frequency will be eliminated in a short time, and the only fields which can oscillate in the resonator are resonant modes.

The electric field and magnetic field can be expressed in terms of a series of frequencies $\{fs\}$ as follows:

$$A(x,y,z,t) = \sum_s \phi_s(x,y,z)e^{j2\pi f_s t}. \tag{1}$$

A can be anyone of the Ex, Ey, Ez, Hx, Hy and Hz.

By taking the discrete Fourier transform, we can change the time-domain field to frequency domain. The Fourier transform of the field shows a local absolute maximum at the frequency f_l which is nearest to the resonant frequency f_0. Following [3], the resonant frequency can be calculated. The Fourier coefficients associated with the frequency f_l at different points of the mesh give the spatial distribution of the electromagnetic fields of the modes under consideration. It can be expressed in rectangular coordinate system as

$$F_{f_l}(i,j,k) = \sum_{n=0}^{N_t-1} A^n(i,j,k,n\Delta t)e^{j2\pi f_l n\Delta t}$$
$$f_l = \frac{l}{N_t\Delta t}, \qquad l = 0, 1, \cdots \frac{N_t}{2} \tag{2}$$

$$\phi_{f_0}(x,y,z) \propto F_{f_l}(x,y,z). \tag{3}$$

Knowing the field distribution, we can calculate the Q-factor of the resonator by incorporating the SIBC or perturbation techniques.

A. FDTD Incorporating SIBC Method

There are two difficulties to compute the Q-factor by the FDTD method. First, it requires a very fine spatial grid to compute the power loss on the conductor wall, which results in a relatively large number of cells for moderately sized objects. Second, the undesirable field is difficult to be removed completely.

The implementation of surface impedance boundary condition can solve the first problem [7]–[10] above. In this work,

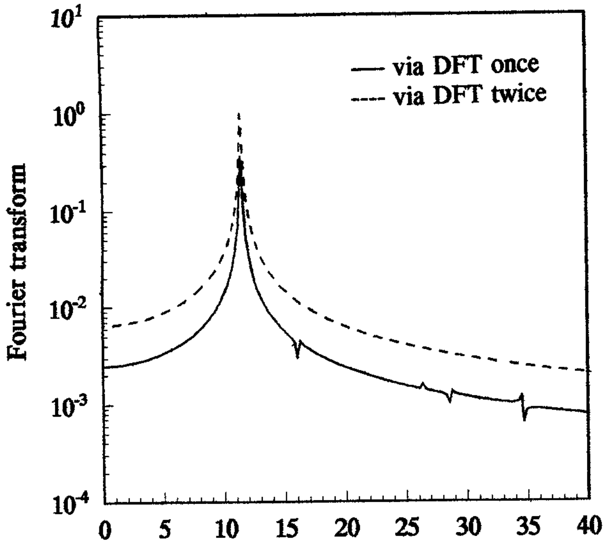

Fig. 1. The spectrum of a typical cylindrical cavity via Fourier transform at TM_{010} mode's resonant frequency.

as we are only concerned with the power loss at the considered frequency, the constant frequency SIBC method is used. The extraction of the considered EM field can be achieved by applying the Fourier transform twice. The process is that we use the distribution of the fields obtained after first time of the Fourier transform as the new exciting fields, and the accurate distribution of the fields can be obtained by taking the Fourier transform once more. Fig. 1 shows the results by applying DFT once or twice. It shows the undesirable field can be up to 1% of the considered field via DFT once. Actually, the remained undesirable field is less than 0.01% after DFT twice.

The equation of the constant frequency SIBC can be written according to [7] as

$$[\mu\Delta_s + L(\Delta_1+\Delta_2)]\frac{dH_t}{dt} + R(\Delta_1+\Delta_2)H_t = -\oint_C E\,dl$$
$$R = R(\omega_0), \quad L = \frac{X(\omega_0)}{\omega_0} \tag{4}$$

where $Z = R + jX$ is the impedance of the conductor wall, Δ_1, Δ_2 is the length of the grid side and Δ_s is the area of the grid as shown in Fig. 2. The values of the electric fields on the conducting wall are set to be zero. Upon substituting

$$\tilde{H} = z_0 H \quad \tilde{R} = \frac{R}{Z_0}$$
$$\tilde{L} = \frac{L}{cZ_0} \quad Z_0 = \sqrt{\frac{\mu_0}{\varepsilon_0}} \tag{5}$$

(4) can be written as

$$\tilde{H}_t^{n+0.5} = C\left(D\tilde{H}_t^{n-0.5} - \frac{c\Delta t}{\Delta_s}\oint_C E\,dl\right) \tag{6}$$

where

$$C = \left[1 + \left(\tilde{L} + \frac{\tilde{R}}{2}c\Delta t\right)\left(\frac{\Delta_1+\Delta_2}{\Delta_s}\right)\right]^{-1} \tag{7}$$

$$D = 1 + \left(\tilde{L} - \frac{\tilde{R}}{2}c\Delta t\right)\left(\frac{\Delta_1+\Delta_2}{\Delta_s}\right) \tag{8}$$

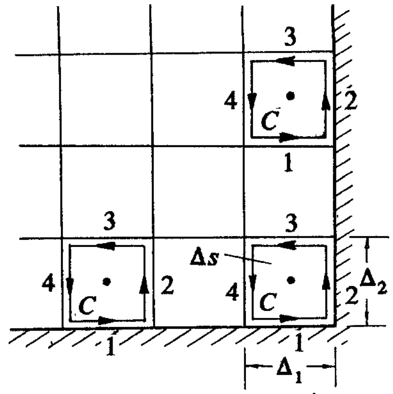

Fig. 2. The contour C to advance H field on the conducting wall.

the closed curve C for the three cases is shown in Fig. 2, in each case the line integral on the conducting wall has been replaced with SIBC.

The loss by dielectric inside the resonator can be calculated by general FDTD algorithm with conductivity σ.

To calculate the Q value of the resonator, we run the program for a time of several periods for considered mode, the initial field is the distribution of electric or magnetic field obtained by lossless FDTD method described as above. Knowing the field values at the beginning and the end of the run time, the Q-factor can be calculated according to definition as follows:

$$Q_0 = 2\pi\frac{W}{W_T} = 2\pi n\frac{A_{t=0}^2}{A_{t=0}^2 - A_{t=nt}^2} \tag{9}$$

it is assumed that the field distribution only change slightly at the end of the run time. A is the maximum value of the field.

The time steps of one period is

$$N_T = \frac{1}{f_0\Delta_t}. \tag{10}$$

B. FDTD Incorporating Perturbation Method

For resonator with high Q value, we can also compute the Q-factor by method of perturbation.

Using the theoretical equations and discritizing its integrations, the Q-factor can be expressed as follows

$$Q_c = \omega_0\frac{W}{P_L} = \frac{2}{\delta}\frac{\int_V \mu|H|^2\,dV}{\oint_s \mu|H_t|^2\,dS} = \frac{2}{\delta}\frac{\sum_{\Delta V}\mu(i,j,k)|F_H(i,j,k)|^2\Delta V}{\sum_{\Delta S}\mu(i,j,k)|F_{Ht}(i,j,k)|^2\Delta s} \tag{11}$$

$$Q_d = \omega_0\frac{W}{P_d} = \omega_0\frac{\int_V \varepsilon|E|^2\,dV}{\int_V \sigma|E|^2\,dV} = \omega_0\frac{\sum_{\Delta V}\varepsilon(i,j,k)|F_E(i,j,k)|^2\Delta V}{\sum_{\Delta V}\sigma(i,j,k)|F_E(i,j,k)|^2\Delta V} \tag{12}$$

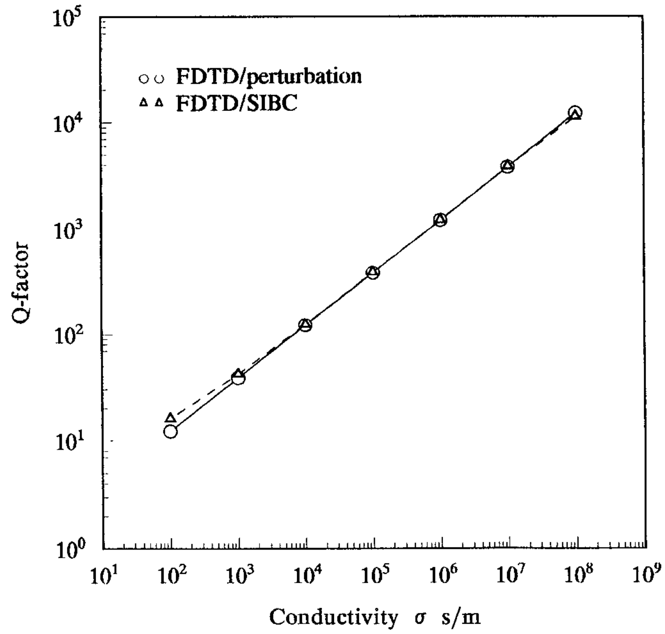

Fig. 3. Q-factor of a parallel-plate resonator versus conductivity of the wall by FDTD/SIBC and FDTD/perturbation method.

where Q_c and Q_d are the Q values only concerned with the conductor loss and dielectric loss separately. W is the maximum stored energy, P_c and P_d are the average dissipated power by conductor wall and dielectric of the resonator, V denotes the volume of the resonator, H_t is the magnetic field tangential to the guide walls and δ is the skin depth of the conductor wall. $F_{E,H}(i,j,k)$ is the Fourier transform value of the field E or H at the point of mesh $s(i,j,k)$, and $F_{Ht}(i,j,k)$ is the Fourier value of the tangential magnetic field on the surface of the conductor wall.

III. Results

A. Two Parallel-Plate Resonator

First we compute the Q-value of a 1-D resonator. We assumed that the length of the resonator was one centimetre which is divided into 100 cells, and $\Delta t = 0.6667$ ps, the time steps of the algorithm $Nt = 2 \times 2^{14}$.

The calculated results for the various conductivity are shown in Fig. 3; and it shows that for $Q > 100$, the results obtained by two methods and the theoretical solutions with perturbation are in close agreement with each other. It is well known that the results obtained by perturbation for both numerical and theoretical methods will have errors for low-Q resonator, because it is assumed that the stored energy is the same during the whole period. Fig. 3 shows that for $Q < 100$, the results by FDTD/SIBC method are bigger than the results with perturbation, the error of the results with perturbation is about 5% for $Q = 50$ and 30% for $Q = 15$. For low-Q resonator, the results by FDTD/SIBC can approximately represent the real values, so it offers obvious advantage over other methods.

The work indicates that the time passed usually has a slight difference with the exact value because of the numerical error when calculating the field value at the end of periods, and this will lead to unacceptable error of the Q-factor. One way to prevent this error is to compute the field values twice with loss or lossless separately and use the values at exactly same time computing the Q-value.

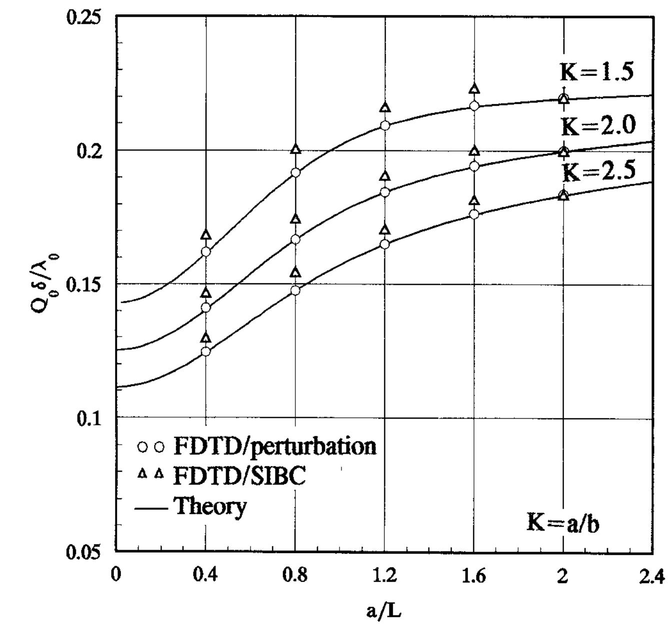

Fig. 4. $Q_0\delta/\lambda_0$ for TE_{101} mode versus the dimension a/L of empty rectangular cavities.

B. Empty Rectangular and Cylindrical Cavities

We have applied the methods to study the Q-factor of TE_{101} mode for an empty rectangular cavity and TE_0 mode for a empty cylindrical cavity. Fig. 4 shows the numerical results of the rectangular cavity. Fig. 5 shows the $Q_0\delta/\lambda_0$ values of TE_0 modes for empty cylindrical cavities with variating D/L. The parameter used are: Total mesh points of 100×150, a time series of 2^{15} and $\Delta t = 0.5 \times \Delta_z$ /c.

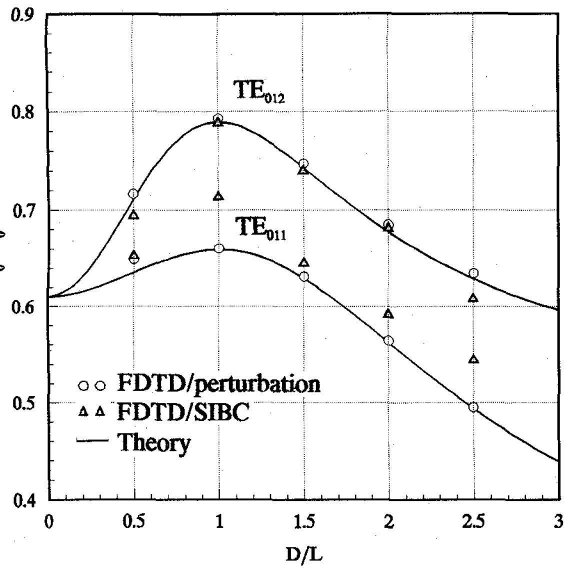

Fig. 5. $Q_0\delta/\lambda_0$ values for TE_0 modes versus the dimension D/L of empty cylindrical cavities.

The numerical results are compared with the theoretical solutions. It shows that the results obtained with the perturbation are more accurate than the results with SIBC method under identical conditions when resonator has a high Q value, and it requires less CPU time to compute Q-factor by equivalent FDTD/SIBC program. Furthermore, it is found that the result-error with perturbation method via the Fourier transform once or twice are within 0.5%, in both cases, the results are in excellent agreement with the theoretical solutions, the error are less than 1%.

For results with SIBC method, their accuracy is greatly influenced by the undesirable modes' fields and the computed field distribution. In these cases, the errors by FDTD/SIBC method are within 5–10%. If more accurate result is expected, more mesh points and CPU time will be needed. So, for resonator with high Q value, FDTD/perturbation method is recommended. As perturbation method has the reasonable discrepancy for studying low-Q resonator, especially, for $Q <$ 100, more accurate results can be obtained by FDTD/SIBC method.

C. Superconductor Sapphire Resonator

We have also studied an extremely high Q resonator formed by a sapphire rod sandwiched by a pair of high Tc superconductor (HTS) films [13] as shown in Fig. 6 using FDTD/perturbation method. The FDTD method can offer the resonant frequency and Q value on all of real boundary conditions. For purposes of comparison, we calculate the resonators described in [13]. Three different size rods are studied with dimensions: 1.000 ″× 0.472″, 0.625″× 0.552″ and 0.197″× 0.098″, (diameter × length) with a pair of 2″-diameter-high-Tc superconductor films.

Table I presents the frequencies obtained by FDTD method according to [3] with permittivity $\varepsilon_r = 9.32$. We have taken the homogeneous space meshes of 101 × 51, 130 × 72, 310 × 31 for three different size rods and a time series of $N = 2^{14}$ instants. The numerical results are in close agreement with

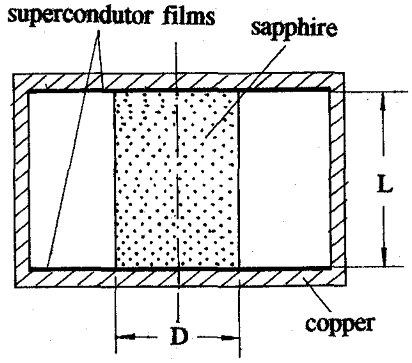

Fig. 6. The structure of a HTS-sapphire-HTS resonator.

TABLE I
RESONANT FREQUENCIES OF THE HIGH Tc SUPERCONDUCTOR-SAPPHIRE RESONATOR (GHz)

Diameter (inch.)	Length (inch.)	Numerical frequency	Results in [13]	Experimental results
1.000	0.472	5.5615	5.552	5.5673
0.625	0.552	6.4682	6.480	
0.197	0.098	27.318	27.33	

TABLE II
UNLOADED Q_0-FACTORS FOR TE_{101} MODE OF A HTS-SAPPHIRE-HTS RESONATOR

T(K)	$R_s(C_u)$ (mΩ)	Numerical results	Solutions in [13]	Experimental result
4.2	3	1.86×10^7	1.4×10^7	
80	10.3	3.71×10^6	3×10^6	
84	10.7	3.30×10^6		3.4×10^6
90	11.5	2.73×10^6	2×10^6	

theoretical values by [13]. The resonant frequency for rod size of 1.000″× 0.472″ obtained by FDTD method is in excellent agreement with the experimental result with $f_0 = 5.5673$ GHz, the error is within 0.1%.

Table II shows the Q_c and Q_d values of the resonator with rod size of 1.000″ (diameter) × 0.472″ (length) at different temperatures. The surface impedance Rs of the superconductor film is obtained by scaling the data in [16] to the resonant frequency according to a f^2 law, the typical values of R_s (copper) at different temperature are used in this case.

The numerical results are in close agreement with theoretical and experimental solutions, although accurate values of the superconductor and copper's surface impedance used in [13] are not known.

As the loss tangent of the sapphire to be $< 10^{-9}$ over the temperature range between 2 and 4.2 K [15], and be $3.5 \times 10^{-17}T^{4.75}$ for temperatures in the range 50–250 K at 9 GHz [14], the numerical result Q_d shows that the dielectric loss can be neglected for this kind of resonator.

It is known that the energy loss on the copper wall can not be neglected because of relatively big value of $R_s(C_u)$, about 500 times the R_s of the superconductor and the larger area of the side wall compare with the area of the superconductor films, even though the magnetic field on the copper wall is very small, about 1/1000 of the maximum field.

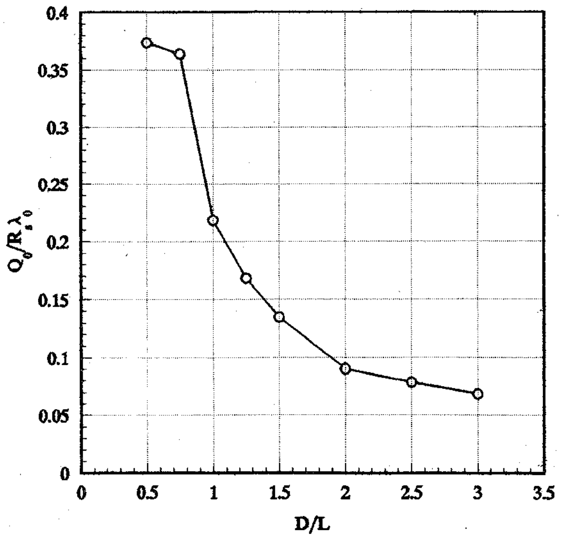

Fig. 7. Q_0R_s/λ_0 values versus the sapphire rod dimension D/L of the HTS shields resonator.

At last, we compute the Q_0R_s/λ_0 values of the resonator with variable size of sapphire rod. It is assumed that the diameter of the cavity is big enough that the loss by side wall can be neglected. The results in Fig. 7 show that high Q value can be achieved with small value of D/L at the same resonant frequency, but small D/L value will cause little difference of the resonant frequencies between TE_{01} and TE_{02} modes. The compromise between high Q-factor and adjacent resonant frequencies should be considered.

IV. Conclusion

We have described the application of the FDTD method to determine the Q-factor of the microwave resonator. It shows that the FDTD/perturbation method is suitable to study the high Q value resonator and FDTD/SIBC method is efficient to study the low Q value resonator. The accuracy is validated by comparing the numerical results with theoretical solutions.

The technique allows to study the resonator with complex structure and wide range of adaptability. With the increasing needs for compact high Q value microwave resonator, it is a very useful and efficient tool for designing and analyzing sophisticated resonators.

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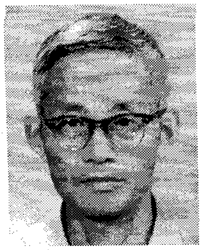

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