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Effect of microstructure on the microwave properties in dielectric ceramics

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Abstract

Electromagnetic simulation of the quality factor measurement was compared to the measurement with a network analyzer. Scattering matrix S_{21} obtained from the network analyzer was compared to the S_{21} obtained from the simulation. From electric field distribution, the dominant resonant $TE_{01\delta}$ mode could be easily determined. The effects of the pore and the conductive inclusion inside the dielectric were investigated. The quality factor decreased with the pore and the second phase in the dielectrics. The decrease of quality factor is more significant when dielectric have conductive inclusions inside the dielectric. Due to the limitations in computer resources and analysis time, the size of the inclusions inside the dielectrics in simulation are not actual size.

Keywords: Cavity resonator; Electromagnetic simulation; Microwave ceramics; Quality factor

1. Introduction

Ceramic dielectrics have been widely studied and applied for the microwave applications such as resonators and filters.[1–4] Recently, the miniaturization of microwave circuit strongly requires high-permittivity low-loss dielectrics with good temperature stability and the tight requirements in communication bandwidth requires high quality factor microwave ceramics. As the measurements of microwave properties becomes more important, many studies have been reported regarding on the measurement environments such cavity and field excitation method. However, in this study, the microstructure of dielectrics and the measurement results will be considered.

Generally, the microwave ceramic dielectrics are fabricated by solid state sintering process with oxide powders. Eventually, imperfections such as pore, grainboundary, and inclusions appear in the microstructure after sintering process. Although there seems to be close relations between the microwave properties and the imperfections in the microstructure, it is very difficult to know the quantitative relations between microstructure and their properties. For example, it is expected that the microwave quality factor decreases with increasing porosity. However, it is difficult to correlate the decrease of quality factor with porosity quantitatively because porous ceramic bodies are likely to have not only physical pore but also imperfect second phase which has different permittivity and dielectric loss. In other words, it is impossible to control independently the porosity, second phase, and inclusions.

Here, we study the correlations between the microstructure and the microwave properties in dielectric ceramics by computer simulation. The simulated results will be compared with measurements by RF network analyzer. From this study, it might be possible to predict the influence of porosity and second phase on the microwave quality factor in a more quantitative manner.

2. Experiments

2.1. Quality factor measurements in the closed metal cavity

There are several methods of determining the dielectric permittivity and the quality facor of microwave dielectrics.[3,5] Among them, cavity resonator method is very useful for the measurement of the quality factor of the dielectrics. Fig. 1 shows the schematic diagram of cavity resonator method. By measuring RF power from

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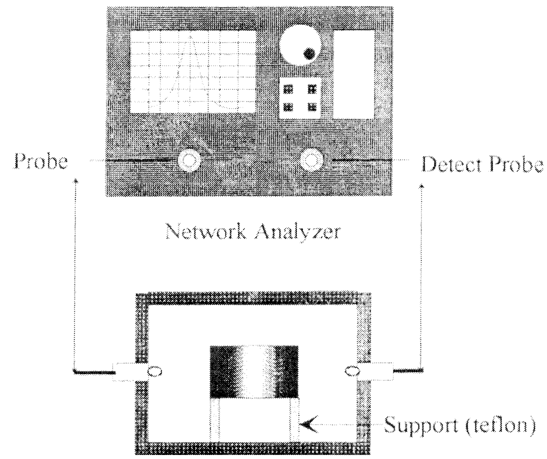

Fig. 1. Schematics of the quality factor measurement in a closed cavity using an RF network analyzer.

port 1 and port 2, scattering matrix S_{21} can be determined. From the plot of S_{21} in frequency domain, the microwave quality factor can be determined by calculating the half-power bandwidth of the peak which appears at dominant resonant frequency.

2.2. Finite element method and HFSS

FEM (finite element method), which had been a very useful numerical method in the field of structural analysis and heat transfer analysis, has been used for electromagnetic analysis since 1968. Compared to FDM (finite difference method) and MoM (method of moment), FEM is more convenient in the analysis of a complicated structure and anisotropic materials.[6–8] Most commercially available 3-dimensional full wave electromagnetic simulators are based on the FEM algorithm. In this study, HFSS (high frequency structure simulator, V7.0, Ansoft Co., USA) was used for the electromagnetic simulation.

HFSS has been widely used for designing RF devices such as filters, resonators, and antenna. HFSS determines electromagnetic vector quantity at every point of interest in the 3-dimensional space, from the complex material values and boundary conditions which are given by users. In HFSS, mesh refinement which requires a complicated algorithm is automatically performed by monitoring the changing rate of the scattering matrix.[8]

3. Results and discussions

3.1. HFSS simulation and experimental measurements of quality factor in BPNT ceramic dielectric

BaO–PbO–$2Nd_2O_3$–$10TiO_2$ (BPNT hereafter) ceramic dielectrics have been widely studied and used for high permittivity microwave applications. HFSS simulation and measurement by the RF network analyzer were compared in BPNT ceramics. For the simulation, materials and physical dimensions of the cavity and dielectric were set up by HFSS setup process. Fig. 2

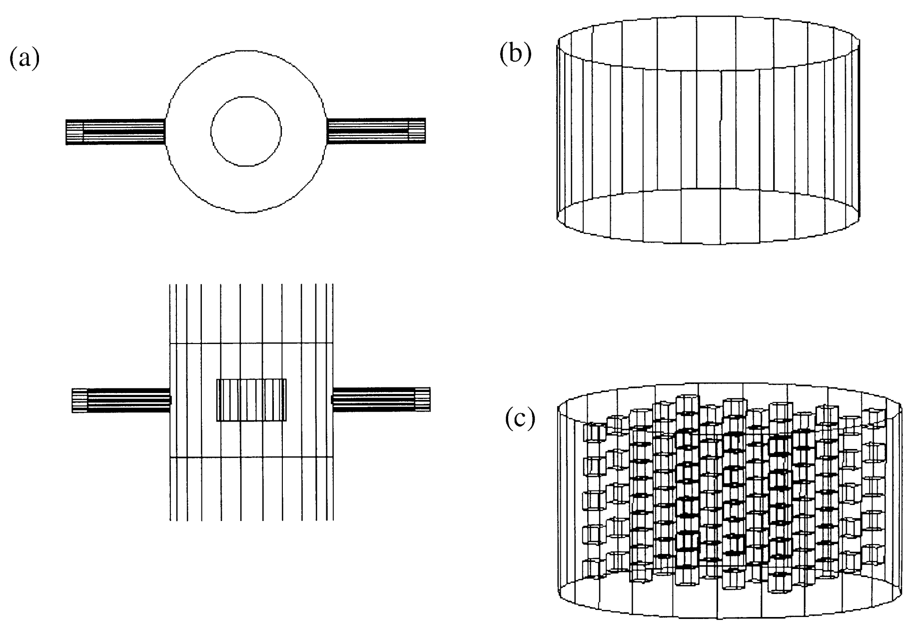

Fig. 2. 3D schematic layout of the metal cavity and dielectric resonator (permittivity of 90 and loss tangent 0.001). Dimensions : cavity height = 20 mm, cavity diameter = 20 mm, resonator height = 10 mm, resonator diameter = 6 mm. (a) Cavity and dielectrics, (b) dielectrics with no inclusions, (c) dielectrics with inclusions such as pore and conductive second phase. Seventy-five cubic incusions, the unit volume of which is 0.5×0.5×0.5 mm are introduced.

shows the schematic diagram of the cavity and the dielectric. The height and diameter of the cavity are 20 mm, respectively. The height and diameter of the dielectrics are 10 and 6 mm. Dielectric is set having permittivity of 90 and loss tangent 0.001.

In the case of the analysis on the pore and inclusions, small cubes are introduced inside the dielectric. Although the actual size of the pores and inclusions are in the μm range, rather large cubes are introduced for rapid simulation. Seventy-five cubic inclusions, the unit volume of which are 0.5×0.5×0.5 mm, are introduced, and therefore, the maximum volume content of inclusions is 2.2%. All metals in Fig. 2 are set as perfect electric conductors.

Fig. 3 shows the scattering matrix S_{21} plots simulated by HFSS and measured by RF network analyzer. In both cases, the $TE_{01\delta}$ mode appears at around 5 GHz. However, overall frequency responses are rather different from each other because material setting for metals and imperfections in the dielectric are neglected in the simulation.

In the measurement, by using the network analyzer, there is no direct method of determining dominant resonant frequency. In the simulation, however, it is possible to find dominant resonant mode by observing the electric field and magnetic field in the dielectrics. Fig. 4 shows electric field vector distributions at selected frequencies in the horizontal plane of the dielectric. From the plots, dominant resonant mode can be easily determined. Referring to the simulated results, it is convenient to determine the dominant resonant frequency in the measurement with a network analyzer.

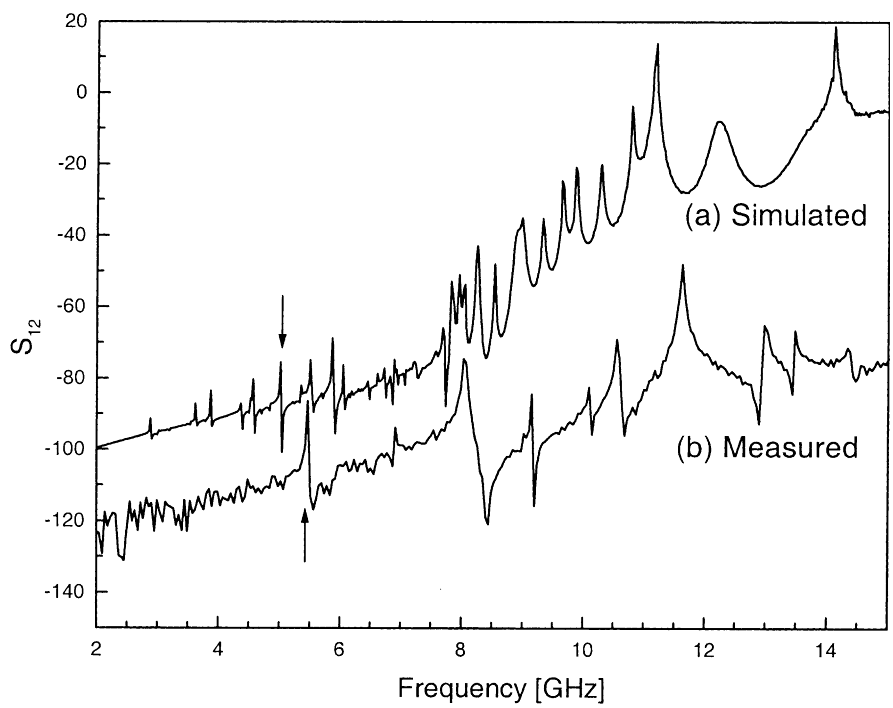

Fig. 3. Frequency dependence of S_{12} in the range of 2–15 GHz. (a) Shows a simulated result using Ansoft HFSS V7.0 and (b) shows measured result using a network analyzer. $TE_{01\delta}$ modes are indicated as arrows.

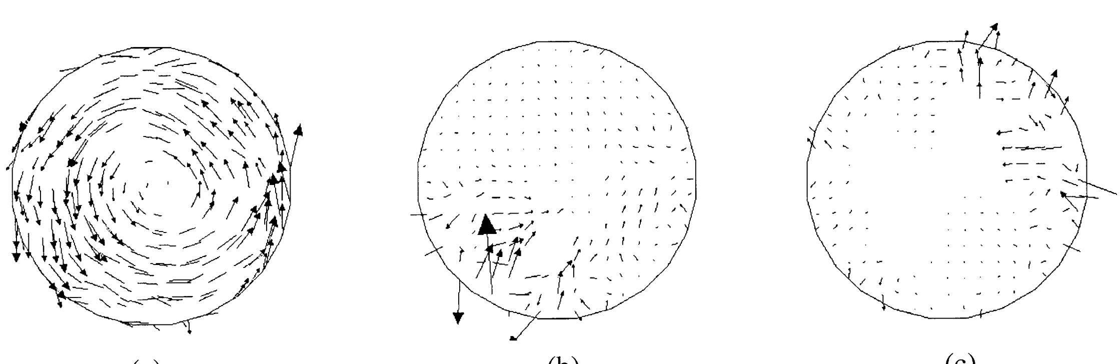

Fig. 4. Vector electric field in the horizontal plane of dielectrics. (a) 5.0 GHz, (b) 5.5 GHz, (c) 5.9 GHz. $TE_{01\delta}$ mode appears at 5.0 GHz.

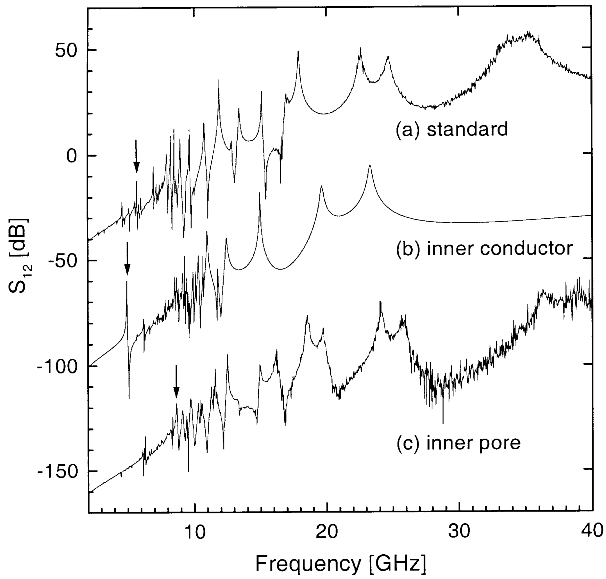

Fig. 5. Frequency dependence of S_{12} in the range of 2–40 GHz. (a) No inclusions in the dielectrics, (b) dielectrics with internal conductive phase, and (c) dielectrics with internal pore. $TE_{01\delta}$ modes are indicated as arrows.

3.2. *Effect of microstructure on the quality factor of dielectric ceramics*

Dielectric ceramics for microwave application are mostly prepared by a solid state sintering process. Eventually, there are imperfections such as pores, grain boundaries, and inclusions in the microstructure. The measured quality factor of the dielectrics is expected to depend on both physical geometry and material properties. However, as it is difficult to control individual microstructure independently, it is also difficult to know the effect of pore and inclusions on the quality factor which is measured by a network analyzer.

Fig. 5 shows the computed frequency dependence of S_{21} with pores and inclusions inside the dielectric. Fig. 5(b) shows the result when dielectrics have no imperfections, Fig. 5(c) shows when dielectrics have pores inside the dielectric, and Fig. 5(a) shows when dielectrics have conductive inclusions inside the dielectric. From the dominant resonant modes in Fig. 5, the quality factors can be calculated as shown in Table 1. When there are imperfections inside the dielectrics, the quality factor decreases. However, the decrease of quality factor is more significant when dielectrics have conductive inclusions inside the dielectric.

Table 1
Calculated unloaded Q when (a) there are no inclusions in the dielectrics, (b) there is a conductor present in the dielectrics, and (c) there is a pore present in the dielectrics

Case	$TE_{01\delta}$ frequency	Unloaded Q
(a) Standard	5.0	840
(b) With conductor	4.0	350
(c) With pore	8.5	810

4. Summary and conclusions

The correlations between the microstructure and the microwave properties in dielectric ceramics are investigated by computer simulation. The simulated results have been compared with measurements by an RF network analyzer. From this study, it might be possible to predict the influence of porosity and second phase on the measured microwave quality factor in a more quantitative manner. From the simulation, it is possible to find a dominant resonant mode easily by observing the electric field and magnetic field in the dielectrics. Where there are imperfections inside the dielectrics, the quality factor decreases. The decrease of the quality factor is more significant when dielectrics have conductive inclusions inside the dielectric. Due to the limitations in computer resources and analysis time, the size of the inclusions inside the dielectrics in simulation are not actual size. Thus, the results in this study should be calibrated through further study.

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