Sample Shape Correction Factors for Cavity Perturbation Measurements

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Convenient analytic expressions for electromagnetic fields inside dielectric objects perturbing a cavity exist only for ellipsoids of rotation. A newly developed code, SEAFISH, was used to calculate sample shape correction factors for cavity perturbation analysis using cylindrical samples with different aspect ratios and complex dielectric constants.

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We have previously derived analytic expressions for perturbation of a cavity by dielectric objects that are ellipsoids of rotation [Hutcheon et al., 1989]. A newly developed code, SEAFISH [de Jong and Adams, 1990], may be used to calculate cavity perturbation by a dielectric object in a cavity, where the object and cavity are arbitrary, coaxial figures of rotation. SEAFISH is a member of the POISSON/SUPERFISH family of codes, which are used extensively in the accelerator physics community [Halbach and Holsinger, 1976]. The code has been used to obtain sample shape correction factors for cylindrical samples with different aspect ratios. Our results suggest a simple experimental calibration technique.

We have reported elsewhere on systems developed for broad studies of microwave permittivity [Hutcheon et al., 1989]. A sample is introduced into the center of a cylindrical microwave cavity. The frequency and Q of the cavity's TM_{010}-mode resonance are measured before and after introduction of the sample. The permittivity of the sample may be derived from these values, the cavity dimensions, and the dimensions of the sample. For a sample whose shape is an ellipsoid of rotation, and whose complex permittivity is ε_r, we showed that the analytic expression for the change in frequency f and quality factor Q as a function of ε_r is

$$\frac{\Delta f}{f_i} + j \bullet \Delta\left(\frac{1}{2Q}\right) = \frac{-\chi_e}{\left(1+\chi_e F_{se}\right)} \bullet \frac{V_s}{V_c} \bullet A \qquad (1)$$

where $\chi_e = \varepsilon_r - 1$, f_i is the initial cavity frequency, V_s and V_c are the sample and cavity volumes, respectively, and where

$$A = \left[\frac{\left|\vec{E}_i\left(\vec{r}_s\right)\right|^2}{2 \bullet \int_{V_c} \left|\vec{E}_i\right|^2 d\left(\frac{V}{V_c}\right)}\right] \qquad (2)$$

is a real, dimensionless calibration constant which depends only on the distribution of the fields in the empty cavity. $\vec{E}_i(\vec{r})$ is the electric field distribution within the unperturbed cavity, and $\vec{E}_i(\vec{r}_s)$ is the unperturbed electric field at the sample location $\vec{r}_s$. Also,

$$F_{se} = \frac{1-e^2}{e^2} \bullet \left[\frac{1}{2e} \bullet \ln\left(\frac{1+e}{1-e}\right) - 1 \right]; \quad e = \sqrt{1 - \frac{b^2}{a^2}} \quad (3)$$

where e is the ellipticity of a sample of length a and diameter b . Given the dimensions of the sample and cavity, we can invert Equation (1) for interpreting cavity perturbation measurements, and may thereby determine the sample permittivity.

The simple application of the derived form of Equation (1) relies on the sample being an ellipsoid of rotation, whereas in practice cylindrical samples are used, with sample holders placed in the cavity to contain and support the sample. Equation (1) also requires that the sample be small relative to the wavelength, whereas larger samples would increase the perturbation of cavity frequency and Q , and would thus improve the accuracy of the permittivity measurement. Equation (1) provides a simple data analysis technique, but it is necessary to know the errors resulting from deviations from the ideal ellipsoid. These errors can only be found using numerical analysis.

Computer Modeling

Using the computer code SEAFISH, one can accurately calculate the frequency and Q of microwave cavities containing lossy dielectrics. The code requires that the cavity and the dielectric elements have rotational symmetry about some axis $\vec{z}$, although they may have arbitrary (r,z) profiles. Our test cavities, including sample and sample holder, have such symmetry. SEAFISH was therefore used to study the validity of the simplifying assumptions in our derivation of Equation (1) and of corrections that might be applied to Equation (1) to improve its accuracy for analyzing data from our measurements.

The study considered the case of an ideal lossless cavity 268 mm in diameter and 88 mm in height. SEAFISH predicts a TM_{010} resonance frequency f_0 of 856.285 MHz for the empty cavity. The TM_{0n0} family of resonances in a simple right-cylindrical cavity may also be found by exact mathematical analysis, since the radial dependence of the rf electric fields is described by the Bessel function $J_0(kr)$. The first root of the Bessel function coincides with the outer radius of the cavity for the TM_{010} mode. This solution predicts a frequency of 856.2875 MHz, and gives the calibration constant A = 1.855 . Note that the SEAFISH frequency prediction agrees well with the exact analysis for this case.

We compared the predictions of Equation (1) with SEAFISH calculations for the case of an ellipsoid of rotation suspended in the test cavity. The ellipsoid was 5.5 mm in diameter and 30 mm in length. The comparison was made for metal and dielectrics with a range of permittivities. The SEAFISH results obtained in the limit of high permittivity approached that for metal, which is shown in Table 1.

TABLE 1
Comparison for Ellipsoidal Samples in TM_{010} Cavity (f_0 = 856 MHz)

Material		SEAFISH δf (MHz)	Equation (1) δf (MHz)
ε'	ε"		
metal	metal	-3.110	-3.073
10	0	-0.941	-0.947
10	10	-1.158	-1.170
26	0	-1.702	-1.699

The frequency-dependent contribution to the imaginary part of the dielectric constant due to a material having a finite conductivity σ is given by

$$\mathrm{Im}(\chi_e) = \varepsilon'' = \frac{\sigma}{2\pi f} \quad (4)$$

using $\varepsilon_r = \varepsilon' - j\varepsilon''$.

For high conductivity material (metal),

$$\lim_{\sigma \to \infty} \frac{-\chi_e}{(1 + \chi_e F_{se})} \bullet \frac{V_s}{V_c} \bullet A$$

$$= \lim_{\chi_e \to -j\infty} \frac{-\chi_e}{(1 + \chi_e F_{se})} \bullet \frac{V_s}{V_c} \bullet A = -\frac{1}{F_{se}} \bullet \frac{V_s}{V_c} \bullet A , \quad (5)$$

which is a real quantity. Thus, the SEAFISH frequency shifts calculated for metal should be the same as in the limiting case of high dielectric constant.

Table 1 shows that the agreement between the frequency shift predicted by SEAFISH and the frequency shift predicted by Equation (1) is within 2%. The shifts in resonant frequency found by SEAFISH are known to be much more accurate than this [de Jong and Adams, 1990], and we infer that the disagreement reflects the effect of assumptions and approximations made in the derivation of Equation (1).

The sample's maximum radius of 2.75 mm represents 4% of the wavelength in a material with $\varepsilon_r = 26$. The electric field at a radius of 0.040 wavelengths from the center of a cavity operating in the TM_{010} mode is 1.6% lower than at the center. This is reasonable uniformity, but may contribute to the discrepancy between the SEAFISH calculations and the simple theory, which assumes that the electric field is constant throughout the region around the sample.

A further comparison was made considering the same cavity excited in the TM_{020} mode, for which the cavity outer radius is at the second root of $J_0(kr)$. The frequency of this mode is 1965.68 MHz, and the calibration constant $A = 4.319$. The results of the calculations are shown in Table 2. We obtain a poorer agreement between Equation (1) and the SEAFISH calculations for this case. With a permittivity of 25 the sample radius represents 9% of a wavelength, at which point the electric field is down 8.5%. The derivation of Equation (1) assumes constant electric field over the sample volume.

TABLE 2
TM_{020}-Mode Comparison (f_0 = 1966 MHz)

Material		SEAFISH	Equation (1)
		δf	δf
ε'	ε"	(MHz)	(MHz)
metal	metal	-18.89	-16.43
25	0	-9.63	-8.92
25	25	-11.50	-10.74

Although Equation (1) and the SEAFISH calculations do not agree perfectly, the frequencies are close enough to make Equation (1) useful for interpreting experimental results. Based on these results, we studied the applicability of Equation (1) to the exact sample and cavity geometry used in our experimental measurements.

SEAFISH calculations were performed for cylindrical samples in a cylindrical hollow quartz sample holder of the type used in our perturbation measurements. These calculations were compared with the results of Equation (1), where F_{se} was evaluated from Equation (3) with the length and diameter of the cylindrical sample as a and b, respectively, but with the exact volume of the cylindrical sample. Differences in frequency shift relative to SEAFISH calculations for several complex permittivities are shown by the crosses plotted in Figure 1.

Application of Equation (1), with these approximations for cylindrical samples in sample holders, differs from the SEAFISH calculations by large amounts over a broad range of ε_r. The approximation of a cylinder by an ellipsoid of rotation is not accurate enough to be useful in analysis of experimental data. The comparison shown in Figure 1 allows us to determine when the approximations are invalid and to develop appropriate calibration techniques.

Calibration Techniques

Note that Equation (1) may be rewritten as

$$\frac{\Delta f}{f_i} + j\Delta\left(\frac{1}{2Q}\right) \approx \left(\frac{\Delta f}{f}\right)_{max} \bullet \frac{\chi_e}{\chi_{se} + \chi_e}, \qquad (6)$$

where

$$\chi_{se} = \frac{1}{F_{se}} \qquad (7)$$

and where

$$\left(\frac{\Delta f}{f}\right)_{max} = -\frac{A}{F_{se}} \bullet \frac{V_s}{V_c}, \qquad (8)$$

which is the limiting value of the fractional frequency shift for very large ε_r. This should be equal to the frequency shift produced by a metal sample of the same dimensions.

Using the more accurate frequencies found using SEAFISH, we can calculate the value of $(\Delta f/f)_{max}$ for the limiting case of a metal sample. This is equivalent to assuming that the electric field is not uniform within the cylindrical sample, and using a reduced "effective" sample volume. Equation (6) may then be normalized to this value of $(\Delta f/f)_{max}$ for data analysis. The results then obtained agree with the SEAFISH values within 2% over a broad range of complex ε_r, as shown by the boxes plotted in Figure 1.

Inverting Equation (6) yields the complex dielectric constant of a sample for which the frequency and Q perturbations have been measured. This method is easily applied to experimental analysis, and the level of agreement obtained is useful for most experimental data.

It is important to note that $(\Delta f/f)_{max}$ is a real value, and may be obtained by calibration with a lossless sample, or by calculations using SUPERFISH, which allows only real dielectric constants [Halbach and Holsinger, 1976]. Equation (6) holds for samples having complex permittivity. The data in Figure 1 were calculated for samples with $\tan(\delta) \leq 1$, and the resulting scatter in the points is less than 3%. Measurements made on metal samples thus provide a simple and reproducible experimental calibration. Since Equation (6) is independent of cavity geometry, we may also extend this method to a cavity

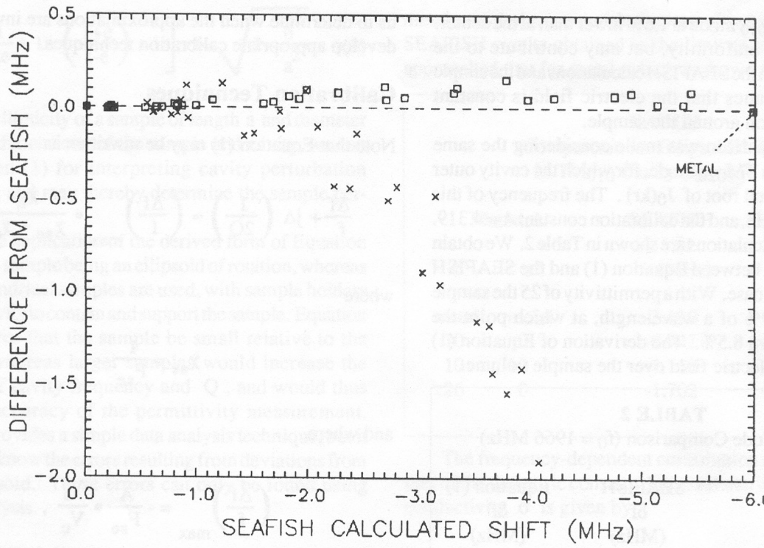

***FIGURE 1:** Differences in frequency shift relative to SEAFISH results. Crosses: Equation (1) evaluated for ellipsoids of the same volume and aspect ratio. Boxes: Equation (6) fitted to SEAFISH calculations for metal.*

of any design having a uniform electric field at the sample. This means that we are not limited to cavity geometries that may be modeled using SEAFISH.

Note that Equation (6) still makes use of Equation (3) for determining the sample shape factor F_{se}, which in turn determines the value of χ_{se}. Equation (3) is not exact for cylindrical samples. Some improvement in accuracy may be obtained by using a value for χ_{se} obtained from a fit to SEAFISH calculations for some intermediate value of ε_r, say $\varepsilon_{cal} = 25$. This can be useful for making measurements on low-loss ($\tan(\delta) \leq 0.3$) samples with error less than 1%.

Solving Equation (6) for the specific case of a calibration sample with a relative dielectric constant of ε_{cal} producing a frequency shift Δf_c, one obtains

$$\chi_{se} = (\varepsilon_{cal} - 1) \bullet \frac{\left(\frac{\Delta f}{f}\right)_{max} - \left(\frac{\Delta f}{f}\right)_{cal}}{\left(\frac{\Delta f}{f}\right)_{cal}}, \quad (9)$$

which may be substituted back into Equation (6) as a calibration constant. The agreement with SEAFISH which may be obtained this way is illustrated by Figure 2. The squares represent the differences in the frequency shifts calculated for several lossless dielectric samples with Equation (6). Values for $(\Delta f/f)_{max}$ and χ_{se} were obtained by fitting to the SEAFISH calculations for, respectively, a metal sample (the last point) and a sample with $\varepsilon_r = 10$ (the sixth point from the left.)

In our measurements of the dielectric properties of materials, we fit $(\Delta f/f)_{max}$ to experimental measurements for metal samples, and fit χ_{se} to experimental measurements for samples made of well-known materials. This allows us to make measurements in a variety of rf cavities driven in a variety of resonant modes, limited by the requirement that the sample size be small relative to the wavelength at the given resonant frequency. The accuracy which we have obtained using this method has been suitable for a wide range of applications [Hutcheon et al., 1989].

Difficulties with this procedure might be expected due to a lack of well-characterized materials with high dielectric constant. For measurements of a given sample, though, the optimum calibration material is one with a dielectric constant a little greater than that of the sample material. It can be seen from Figure 2 that this minimizes the expected error.

Samples of high-quality polytetrafluoroethylene (PTFE) and fused silica serve well as calibration samples for measurements of small ε_r. Oriented single-crystal sapphire should

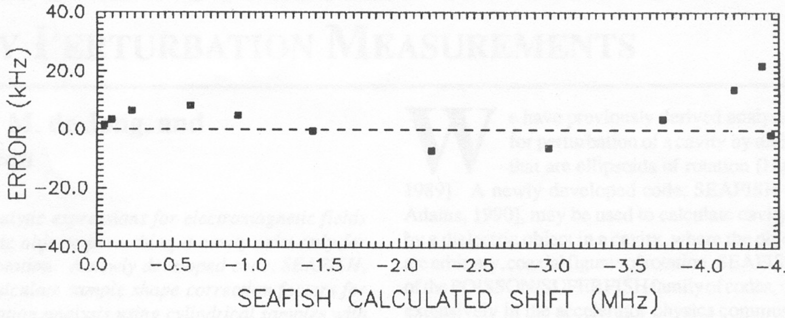

***FIGURE 2:** Residual error after fitting Equation (4) to SEAFISH calculations at $\varepsilon = 10$ and at limit of large ε for lossless dielectrics.*

serve well for measurements up to $\varepsilon_r = 10$. Beyond this value, we use SEAFISH calculations for calibrating our measurements.

Conclusions

The computer code SEAFISH was used to determine the use of cavity perturbation techniques for studying dielectric materials in cylindrical samples. A simple experimental calibration technique using copper calibration samples was developed to allow the measurement of the complex permittivity to within 5%. Better accuracy (error < 1%) may be obtained by a further calibration step, using either well-characterized samples or SEAFISH (or SUPERFISH) calculations.

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