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Restoration of the Lorentzian and Debye Curves of Dielectrics and Magnetics for FDTD Modeling

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RESTORATION OF THE LORENTZIAN AND DEBYE CURVES OF DIELECTRICS AND MAGNETICS FOR FDTD MODELING

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Abstract –The algorithms of extracting the Lorentzian- and Debye-curve parameters of dielectric and magnetic materials from the results of measurements at several frequency points are presented. These algorithms are based on an analytical solution of systems of non-linear equations with physical constraints that follow from the fundamental principle of causality. The extracted parameters are useful for FDTD modeling of electromagnetic structures containing such dispersive media. Some examples are presented.

I. INTRODUCTION

Structures containing dispersive materials, including novel composite media for various EMC applications, can be effectively modeled using the FDTD technique. Linear dispersive materials can be treated by recursive time-domain convolution of magnetic or dielectric susceptibility and corresponding field components [1]. However, to fulfill this, the corresponding frequency-domain susceptibility must have a causal Fourier (or Laplace) transform that contains a sum of complex exponential functions of time. The simplest example is a Debye model for comparatively low-frequency (from RF, UHF to the lower part of microwave band) behavior of a dispersive medium associated with dipolar polarization of molecules in dielectrics, or with domain wall movement in magnetic materials. At higher frequencies (from microwaves and mm-waves to IR, visible, and UV waves) resonance effects are due to ionic and electronic polarizability in dielectrics, and electron spin magnetic moments precession in magnetic media [2]. These effects can be taken into account by a Lorentzian model. A general equation for a single-pole Lorentzian dispersion law for the permittivity of a single-component material is

$$\varepsilon(f) = \varepsilon_\infty + \frac{A}{1 + jf/f_{rel} - (f/f_0)^2} - \frac{j\sigma_e}{2\pi f \cdot \varepsilon_0}, \qquad (1)$$

where amplitude parameter is $A = \varepsilon_S - \varepsilon_\infty$; ε_S and ε_∞ are static dielectric constant and optic region permittivity; f_0 is the resonance frequency. The relaxation frequency parameter is $f_{rel} = f_0^2 / \Delta f$, where Δf is the width of the Lorentzian resonance line at –3 dB level. The second term in (1) is the frequency-domain susceptibility function responsible for polarization of the dielectric molecules. The last term in (1) takes into account the conductivity loss in the material, σ_e is the d.c. electric conductivity of the material, and ε_0 is the permittivity of free space.

The Debye dispersion law is a particular case of the more general formula (1) when $f_0 \to \infty$,

$$\varepsilon_r = \varepsilon_\infty + \frac{A}{1 + jf/f_{rel}} - \frac{j\sigma_e}{2\pi f \varepsilon_0}. \qquad (2)$$

The relaxation frequency is $f_{rel} = 1/(2\pi\tau)$, where τ is the Debye loss constant, which is a characteristic property of each material.

The dispersion law for the Lorentzian magnetic material permeability is written in the similar way as (1),

$$\mu(f) = 1 + \frac{A}{1 + jf/f_{rel} - (f/f_0)^2}, \qquad (3)$$

but there is no term associated with conductivity. The resonance amplitude parameter *A* for the magnetic material depends on the type of the magnetic material. For the Debye magnetic material the last term in denominator of (3) is omitted.

In most cases parameters of Lorentzian or Debye curves for dielectric or magnetic materials are unknown, but some reference and experimental data are available. Frequently, measurements are fulfilled using narrowband cavity techniques to increase the sensitivity, and the data only in a few frequency points are available [3]. The Debye or Lorentzian parameters can be extracted from these data using the algorithms described below.

However, in actual materials the dispersion curves are frequently of more complex shape. In dielectrics, the Cole-Cole dispersion law or its modifications result in smoother frequency dispersion than the Debye model [4]. In magnetic materials, complex magnetic spectra with multiple Lorentzian lines are typical [5]. In these cases, introduction of the conductive term in the generalized dispersion law allows distortions of the dispersion curves to be fit within a finite frequency range while retaining a rational form of the law that is of importance for FDTD applications.

II. THE LORENTZIAN MODEL

Extracting the Lorentzian model parameters from measurements is based on solving a system of non-linear equations. The frequency–domain susceptibility function for a dielectric in (1) or magnetic in (3) is complex,

$$\chi(f) = \chi'(f) - j\chi''(f)\,, \qquad (4)$$

and its real and imaginary parts are

$$\chi'(f) = \frac{A\left(1-(f/f_0)^2\right)}{\left(1-(f/f_0)^2\right)^2 + (f/f_{rel})^2} \qquad (5)$$

and

$$\chi''(f) = \frac{A(f/f_{rel})}{\left(1-(f/f_0)^2\right)^2 + (f/f_{rel})^2}\,. \qquad (6)$$

There is no necessity to measure exactly the resonance line width, resonance frequency and corresponding resonance amplitude. It is sufficient to have suitably accurate measurements of χ' or χ" at three frequency points, with at least two points at different slopes of the resonance curve. The imaginary part of susceptibility associated with attenuation is usually measured at microwave frequencies by means of a waveguide or cavity technique [3]. In this case, the three measured values of χ'' at three frequencies are, correspondingly,

$$\begin{cases} \chi''_1 = \dfrac{A(f_1/f_{rel})}{\left(1-(f_1/f_0)^2\right)^2 + (f_1/f_{rel})^2} \\ \chi''_2 = \dfrac{A(f_2/f_{rel})}{\left(1-(f_2/f_0)^2\right)^2 + (f_2/f_{rel})^2} \\ \chi''_3 = \dfrac{A(f_3/f_{rel})}{\left(1-(f_3/f_0)^2\right)^2 + (f_3/f_{rel})^2} \end{cases}. \qquad (7)$$

This system of three non-linear equations with three unknowns can be solved analytically. However, since the analytical solution is cumbersome, a MATLAB program was developed to apply physical constraints on the region of possible solutions. Only physically reasonable solution satisfying the following conditions is permitted:

- the values A, f_{rel}, and f_0 are real and positive;
- the resultant resonance frequency satisfies either $f_1 < f_0 < f_2$, or $f_2 < f_0 < f_3$.

This method of extracting parameters for the Lorentzian curves deals with susceptibility and can be applied to magnetic media. As for dielectrics, when the d.c. conductivity σ_e is not taken into account, four equations are needed to find f_{rel}, f_0, static dielectric constant ε_s, and optical permittivity ε_∞. These may be measurements of both real and imaginary parts of susceptibility at two frequency points. Additional conditions when solving such a system are that ε_S and ε_∞ are real and positive, and $\varepsilon_S > \varepsilon_\infty$. In many cases, the single-pole Lorentzian dielectric media that exhibit substantial loss at high frequencies is of interest, and the d.c. conductivity can be neglected.

However, if the conductivity term contributes significantly, then five equations are needed for extracting five unknowns (f_{rel}, f_0, σ_e, ε_S, and ε_∞). The conductivity σ_e is required to be real and positive. The system of equations then, for example, is the following:

$$\begin{cases} \chi''_1 = \dfrac{(\varepsilon_S - \varepsilon_\infty)(f_1/f_{rel})}{\left(1-(f_1/f_0)^2\right)^2 + (f_1/f_{rel})^2} - \dfrac{\sigma_e}{2\pi f_1 \varepsilon_0} \\ \chi''_2 = \dfrac{(\varepsilon_S - \varepsilon_\infty)(f_2/f_{rel})}{\left(1-(f_2/f_0)^2\right)^2 + (f_2/f_{rel})^2} - \dfrac{\sigma_e}{2\pi f_2 \varepsilon_0} \\ \chi''_3 = \dfrac{(\varepsilon_S - \varepsilon_\infty)(f_3/f_{rel})}{\left(1-(f_3/f_0)^2\right)^2 + (f_3/f_{rel})^2} - \dfrac{\sigma_e}{2\pi f_3 \varepsilon_0}\,. \\ \chi'_1 = \dfrac{(\varepsilon_S - \varepsilon_\infty)\left(1-(f_1/f_{rel})^2\right)}{\left(1-(f_1/f_0)^2\right)^2 + (f_1/f_{rel})^2} \\ \chi'_2 = \dfrac{(\varepsilon_S - \varepsilon_\infty)\left(1-(f_2/f_{rel})^2\right)}{\left(1-(f_2/f_0)^2\right)^2 + (f_2/f_{rel})^2} \end{cases} \qquad (8)$$

If the number of experimental data available is larger than the number of unknown parameters, the accuracy of the dispersion curve reconstruction can be improved. The system of equations can be solved for all possible combinations of the experimental data (points) when the number of points is equal to the number of the unknowns. Then, averaging of all these results allows minimizing the uncertainty of the reconstructed parameters.

III. RANDOM MEAN SQUARE METHOD FOR THE LORENTZIAN CURVE RESTORATION

If the dispersion law of a material is characterized by a single pole, i.e. includes a single frequency-dispersive term, then another technique for the reconstruction of the parameters of dispersion curve is available. In this case, only the data on the dielectric loss is exploited which requires twice as much experimental data. This method of reconstruction is less cumbersome and more straightforward.

The frequency dependence of the imaginary part of permittivity following from the general normalized Lorentzian form (1) with omitted d.c. conductivity is

$$\varepsilon''(f) = \frac{A f/f_{rel}}{\left(1-(f/f_0)^2\right)^2 + (f/f_{rel})^2} \,. \tag{9}$$

A new set of parameters *x*, *y* can be introduced as

$$x = f^2, \quad y = f/\varepsilon'' \tag{10}$$

From (9) and (10) it follows that *y* is a quadratic function of *x*,

$$y = ax^2 + bx + c \tag{11}$$

with

$$a = \frac{f_{rel}}{A f_0^4}, \quad b = \frac{f_{rel}}{A}\left(\frac{2}{f_0^2} - \frac{1}{f_{rel}^2}\right), \quad c = \frac{f_{rel}}{A} \tag{12}$$

To find the parameters for the Lorentzian curve, the experimental data are fit to the quadratic function (11). The fit uses the random mean square method, which involves searching the parameters of the quadratic dependence by solving the system of linear equations:

$$\begin{cases} \alpha_2 a + \alpha_1 b + \alpha_0 c = \beta_0 \\ \alpha_3 a + \alpha_2 b + \alpha_1 c = \beta_1 \\ \alpha_4 a + \alpha_3 b + \alpha_2 c = \beta_2 \end{cases} \tag{13}$$

with

$$\alpha_k = \frac{1}{n}\sum_i x_i^k \quad \text{and} \quad \beta_k = \frac{1}{n}\sum_i y_i x_i^k \tag{14}$$

and x_i and y_i are related by (11) to the i-th of n available experimental data. The best fit for the parameters a, b, and c is given by the solution of system (13). Once these parameters are known, the parameters of the dispersion curve, namely A, f_0, and f_{rel} can be found from (12). To find the optical permittivity, ε_∞, data on the real part of permittivity are necessary.

This technique was applied to process the frequency dependence of the transmission coefficient obtained in a permittivity measurement with the resonance cavity [6].

IV. THE DEBYE MODEL

A method for extracting the Debye dielectric parameters with low-frequency conductivity losses using measurement data at two frequency points is described in [7]. The system of four non-linear equations for $\varepsilon'(f_1)$, $\varepsilon''(f_1)$, $\varepsilon'(f_2)$, and $\varepsilon''(f_2)$ is solved numerically, however, there is a problem with the solution convergence. To obtain the solution, some approximation factors K_i (i=1…4) are introduced in [7]. However, the resultant system of non-linear equations is unstable with respect to the factors K_i . Even less than 0.1% variation in K_i can result in impossibility to converge to a solution.

A new method, free from this convergence problem described here, is based on a direct analytical solution of a system of equations and application of physical constraints.

The system of the equations for the Debye dielectric with a conductivity term is the following:

$$\begin{cases} \varepsilon_1' = \varepsilon_\infty + \dfrac{A}{1+(f/f_{rel})^2} \\ \varepsilon_2' = \varepsilon_\infty + \dfrac{A}{1+(f/f_{rel})^2} \\ \varepsilon_1'' = -\dfrac{A(f/f_{rel})}{1+(f/f_{rel})^2} - \dfrac{\sigma_e}{2\pi f_1 \varepsilon_0} \\ \varepsilon_2'' = -\dfrac{A(f/f_{rel})}{1+(f/f_{rel})^2} - \dfrac{\sigma_e}{2\pi f_2 \varepsilon_0} \end{cases} \,. \tag{15}$$

The restrictions are that all the unknown solutions (A, ε_∞, σ_e, f_{rel}) must be real and positive; if $f_1<f_2$, then $\varepsilon'(f_1) > \varepsilon'(f_2)$, and since loss tangents are $\tan\delta(f_1) < \tan\delta(f_2)$, $\varepsilon''(f_1)\varepsilon'(f_2) < \varepsilon'(f_1)\varepsilon''(f_2)$,

The system (15) is solved analytically by the ordered elimination method of variables, and the MATLAB program, analogous to that described in Section II, selects regions of physically possible solutions at every elimination step.

The relaxation Debye frequency f_{rel} is derived from (15) in a simple form

$$f_{rel} = \frac{\varepsilon_1'' \cdot f_1 - \varepsilon_2'' \cdot f_2}{\varepsilon_2' - \varepsilon_1'} \,. \tag{16}$$

The conductivity is calculated as

$$\sigma_e = 2\pi f_1 \varepsilon_0 \left\{ \varepsilon_1'' + \frac{f_1 f_{rel}}{f_1^2 - f_2^2} (\varepsilon_1' - \varepsilon_2') \cdot \left(1 + \left(\frac{f_2}{f_{rel}} \right)^2 \right) \right\}, \quad (17)$$

and the optical and static permittivity values, correspondingly, are

$$\varepsilon_\infty = \frac{\varepsilon_1' - \varepsilon_2' + \varepsilon_1' \cdot (f_1 / f_{rel})^2 - \varepsilon_2' \cdot (f_2 / f_{rel})^2}{(f_1 / f_{rel})^2 - (f_2 / f_{rel})^2} \quad (18)$$

$$\varepsilon_S = \varepsilon_1' + (\varepsilon_1' - \varepsilon_\infty) \cdot (f_1 / f_{rel})^2 \quad (19)$$

A similar procedure can be done for Debye magnetic materials.

V. EXAMPLES

Example 1.

Extraction of the Lorentzian-curve parameters can be demonstrated using some experimental data for electrodynamically isotropic powder of an M-type Barium hexagonal ferrite:

$$f_1 = 5\,\text{GHz}; \quad \chi_1'' = 1.2;$$
$$f_2 = 8\,\text{GHz}; \quad \chi_2'' = 2.0;$$
$$f_3 = 15\,\text{GHz}; \quad \chi_3'' = 0.8.$$

The parameters for the Lorentzian curve are A=3.82, f_0=10.1 GHz, and f_{rel}= 99.03 GHz, which corresponds to the width of the ferrite resonance line Δf=1.03 GHz.

Since for the hexagonal ferrite the parameters of the Lorentzian curve are related to the physical parameters as [8]

$$f_0 = f_A = \frac{\mu_0 \cdot \gamma \cdot H_A}{2\pi}, \quad (20)$$

$$A = M_S / H_A, \quad (21)$$

and

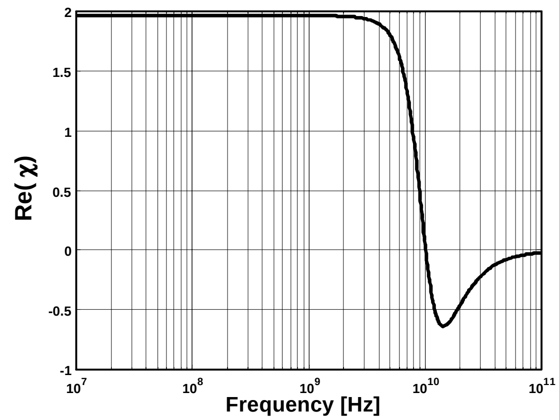
$$\Delta f = \frac{f_0^2}{f_{rel}} = \frac{\mu_0 \cdot \gamma \cdot \Delta H}{\pi}, \quad (22)$$

where $\mu_0 = 4\pi \cdot 10^{-7}$ H/m is permeability of vacuum, $\gamma = 1.76 \cdot 10^{11}$ C/kg is the gyromagnetic ratio, H_A is the crystallographic anisotropy field, ΔH is the resonance line width in terms of magnetic field, and M_S is the saturation magnetization of the hexagonal ferrite.

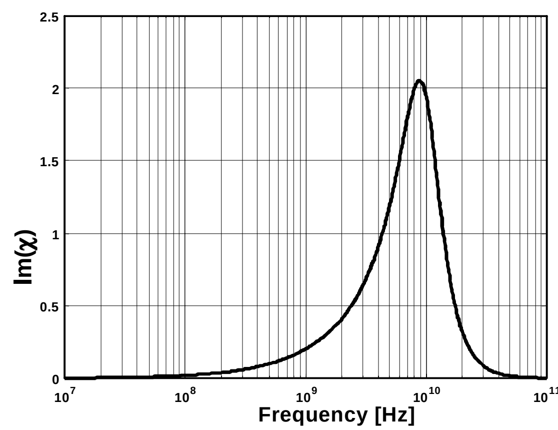
The extracted parameters of the Lorentzian curve correspond to the physical parameters of the hexagonal ferrite:

- $H_A = 2.87 \cdot 10^5$ A/m= 3.57 kOe;
- $\Delta H = 1.48 \cdot 10^5$ A/m = 1.85 kOe;
- $M_S = 5.65 \cdot 10^5$ A/m; $4\pi M_S = 88.4$ kGs.

The extracted frequency dependencies are shown in Figure 1 (a, b).



(a)



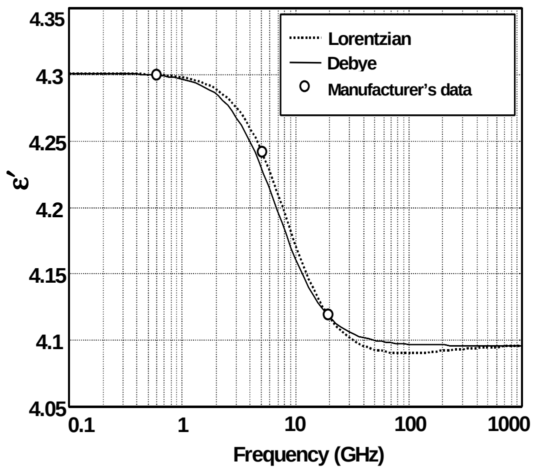
(b)

Figure 1. Extracted curves for the M-type Barium hexagonal ferrite: (a) real part; (b) imaginary part of magnetic susceptibility.

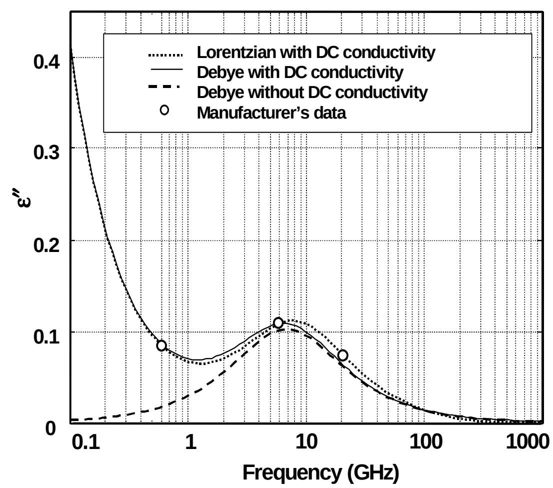
Example 2.

The parameters of the dispersion curves for the dielectric FR-4 used in the printed circuit boards are obtained from the manufacturer's data, as described in Sections II. For the Lorentzian model the extracted parameters are ε_s=4.301; ε_∞=4.096; $\sigma_e = 2.294 \cdot 10^{-3}$ S/m, f_0=39.5 GHz; Δf =200 GHz. For the corresponding Debye model the parameters are ε_s =4.301, ε_∞=4.096, $\sigma_e = 2.294 \cdot 10^{-3}$ S/m, $\tau = 2.294 \cdot 10^{-11}$s. The corresponding frequency characteristics are shown in Figure 2 (a, b).

A two-sided copper-clad board having the dimensions 200x150 mm used in S-parameters measurements and FDTD modeling that allowed taking into account Lorentzian dispersion of the dielectric, is shown in Figure 3. Positions of Ports 1 and 2 are indicated in mm. Figure 4 shows the FDTD modeled and measured frequency dependence of $|S_{21}|$ for the test board with the described above dielectric. The measured and FDTD modeled results agree well in the frequency range up to 5 GHz, and this indicates that the parameters of the dielectric are extracted correctly.



(a)



(b)

Figure 2. Debye and Lorentzian dielectric models of a test substrate containing FR4: (a) real part of permittivity, and (b) imaginary part of permittivity.

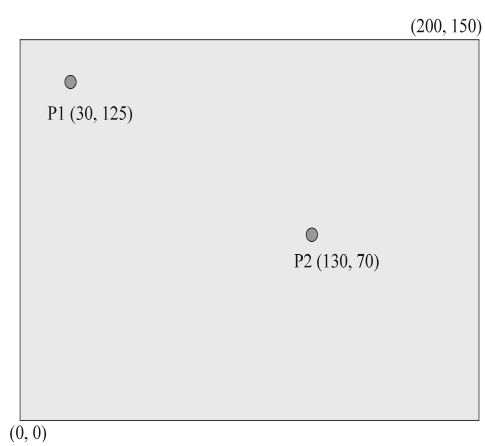


Figure 3. Schematic of the test double-sided copper cladded substrate with dispersive dielectric in between.

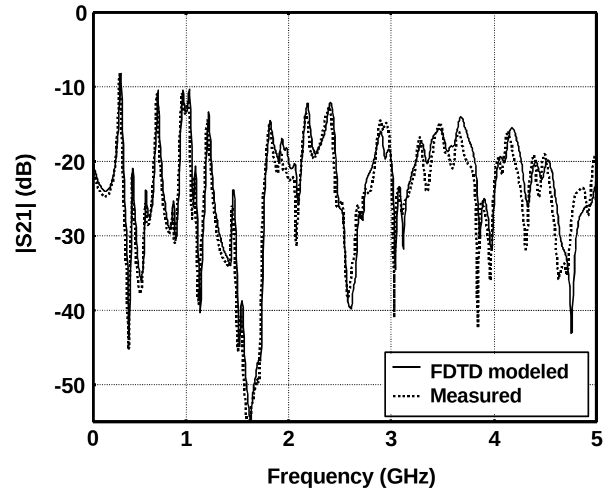
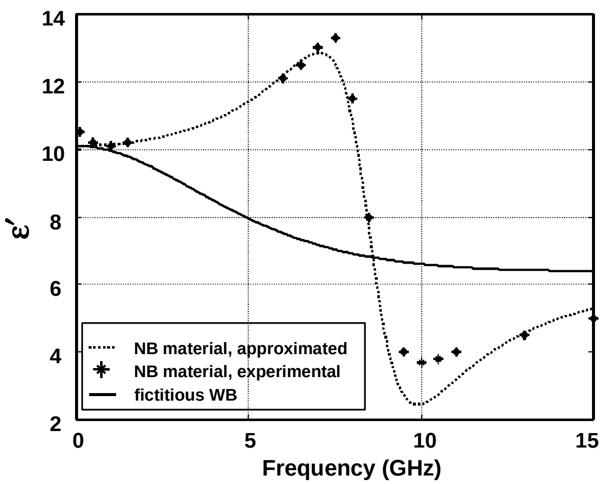


Figure 4. The FDTD modeled and measured $|S_{21}|$ parameter for a double-sided PCB with FR-4 dielectric.

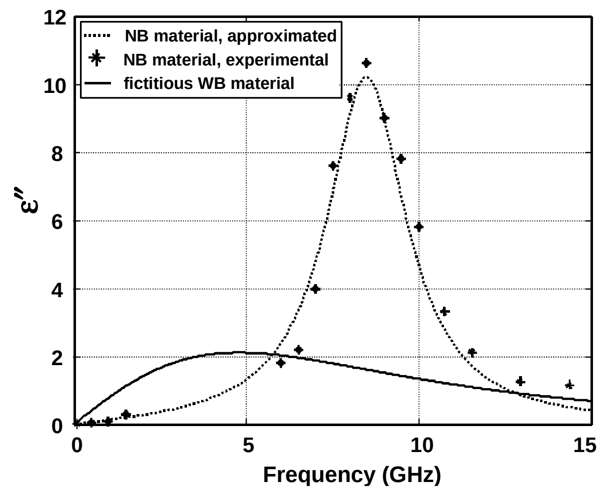
Example 3.

Experimental frequency characteristics of the narrowband (NB) composite dielectric Lorentzian material [9, Fig. 7(a, b)], approximation curves, as well as the characteristics of some fictitious wideband (WB) Lorentzian material are presented in Figure 5 (a, b). The extracted parameters for the NB material obtained by the random mean square method are ε_s=10.1, ε_∞=6.8, f_0=8.6, Δf=2.8 *GHz*. The fictitious WB material, the frequency characteristic of which is also presented in Figure 5, has the same parameters as the NB material, except that the width of the resonance line is Δf=17.8 GHz.

WB and NB Lorentzian materials differ by the ratio of the half-width of the resonance curve at –3 dB level to the resonance frequency. When $\Delta f/(2f_0) \geq 1$, it is a wideband Lorentzian material with frequency characteristics similar to the Debye model, as shown in Figure 2 (a,b) for FR-4. When $\Delta f/(2f_0) < 1$, it is a narrowband Lorentzian material suitable for resonance effects and highly absorbing media modeling. For modeling WB and NB materials, different recursive convolution procedures in FDTD should be used, as shown in [10]. The NB or WB materials in FDTD modeling were placed between two perfect electric conductor (PEC) planes to compose the same test board as shown in Figure 3. The frequency dependence of the S-parameters of the test board over the frequency range from 0 to 15 GHz is presented in Figure 6 (a, b). The figure demonstrates the possibility of a stop-band filter design based on the NB material that has the extracted parameters.



(a)



(b)

Figure 5. Permittivity for the Lorentzian narrowband and wideband dielectrics: (a) the real part, and (b) the imaginary part.

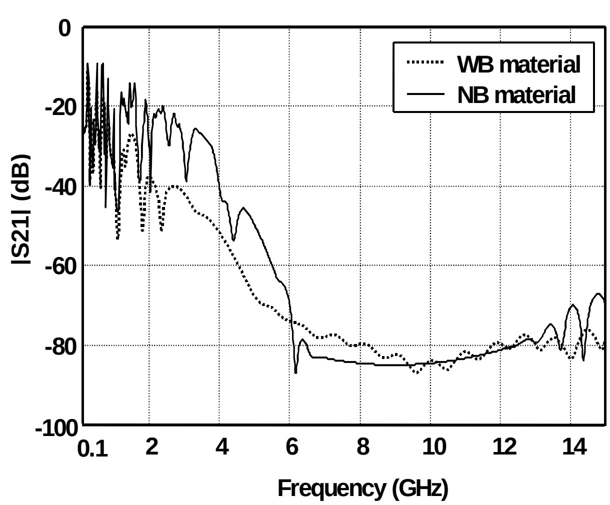


Figure 6. FDTD modeled $|S_{21}|$ results for a wideband and a narrowband Lorentzian dielectrics.

VI. CONCLUSIONS

Algorithms and numerical examples of extracting the Lorentzian and Debye curves for dielectric and magnetic materials are based on the solution of systems of non-linear equations with physical constraints that follow from the fundamental principle of causality. For a Lorentzian curve just three frequency points are enough, so that at least one of the points would be on each slope of resonance curve. For the Debye dielectric model with conductivity loss, real and imaginary parts of permittivity at just two frequency points on different sides of the resonance curve should be known. The extracted parameters are useful for FDTD modeling of electromagnetic structures containing such dispersive media.

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