Communication

Stochastic Polynomial Chaos Expansion Analysis of a Split-Ring Resonator at Terahertz Frequencies

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Abstract—**Polynomial chaos expansion (PCE) technique is applied to a conducting array of split-ring resonator to study the effect of the uncertainties of its design parameters on its reflectance at terahertz frequencies. The uniformly distributed random input design parameters have been considered. The first (average) and second (standard deviation) moments are estimated using the PCE. Strong variation of the output response caused by the uncertainties of the design parameters has been noticed. A sensitivity analysis has been carried out to assess the influence of each input parameters on the reflectance. The results show the effectiveness of the PCE and demonstrate that the PCE can be a useful statistical tool to analyze electromagnetic structures.**

Index Terms—**Metamaterials (MMs), polynomial chaos expansion (PCE), split-ring resonator (SRR), statistical analysis.**

I. Introduction

Over the past decades, a relatively new domain in electromagnetics (EMs) called metamaterials (MMs) has emerged. This new concept enabled scientist and engineers to tailor, at least theoretically, new materials and components with fascinating properties. Split-ring resonators (SRRs) that are an important part of MMs have been widely investigated. It has been demonstrated both numerically and experimentally that a periodically arranged conducting SRRs over a substrate exhibit negative permeability around the magnetic resonance [1]. Depending on the frequency of application, the dimensions of the SRR can span from centimeter for microwaves (MWs) to micrometer for terahertz (THz) frequencies. First proposed by Pendry *et al.* [2], an SRR is usually formed by two concentric loops of conducting material etched on a substrate. A small portion of the loops is cut off to form a slit situated on opposite sides of the loops. The presence of the slits is of capital importance since they allow the structure to resonate at higher wavelengths (lower frequencies) compared to its physical dimensions. The SRR can be considered as an oscillating LC circuit composed of a magnetic coil of inductance L and a capacitance of C. The slits act as parallel plate capacitors while the conducting loops act as inductors.

The magnetic resonance of the SRR appears when the incident time-varying EM field has a magnetic field component penetrating the SRR plane (magnetic field perpendicular to the plane of the SRR). Thus, this TE polarization mode couples with the capacitance of the loops and induces a current around the SRR. This induced current produces in turn a magnetic field which interacts with the external field and generates the magnetic resonance [3]. The magnetic response depends closely on the design parameters such as the gap size, the lattice period, and the ring length. In [4], many studies on the effect of these parameters on the desired EM response can be found, but these works focused mainly on the effect of some design parameters with limited number of trials that are not sufficient in term of statistics, i.e., probability density function (PDF), average value, and variance. The design parameters can be considered to be variables having uncertainties due to the process of fabrication and environmental conditions. The evaluation of the effect of the variability of these design parameters on the output response is usually performed using statistical approaches. Monte Carlo (MC) simulations are universal approaches that can estimate with accuracy the distribution of the output response based on the PDF attributed to the random design parameters. They rely on the repeated random selection of the design parameters to compute the corresponding output response. However, MC technique may require high number of samples in order to obtain high confidence in the desired output response. Despite the popularity of the MC technique, it is thus not suitable for large problems. On the other hand, polynomial chaos expansion (PCE) has become attractive in many engineering fields due its powerful capabilities in estimating complex models with reasonably low number of sampling data. So far, the PCE has been successfully applied in the field of engineering such as mechanics [5], [6], nuclear engineering [7], and fluid dynamics [8]. Chauvière *et al.* [9] are among the first to use PCE in computational EMs. Later, a multielement probabilistic collocation method based on the use of the PCE has been proposed by Yücel *et al.* [10] to analyze a transmission line network. One has also to mention the work carried out by Austin and Sarris [11] on the finite-difference time domain method using PCE applied to MW circuits. Other works related to PCEs exist in [12]–[15]. This communication deals with the application of the statistical PCE for the study of the SRR for which some of the geometrical dimensions are considered to be random variables and their impact on the reflectance (output response) is studied. We believe that this communication may be useful for engineers designing SRRs where small variations of the geometrical parameters are of capital importance for the device performances.

II. Results and Discussion

An array of SRR consisting of two concentric conducting square loops has been considered. The SRR is of copper with conductivity $\sigma = 5.8\times100^{7}$ S/m and it is placed on a quartz substrate with 3.78 as dielectric constant. The SRR array along with the substrate is shown in Fig. 1(a). The unit cell [Fig. 1(b)] of the periodic array is investigated using the commercial EM software HFSS to simulate the magnetic response of the SRR structure. The SRR deposited on the quartz substrate is illuminated with a normally incident EM plane wave. Floquet ports are assigned on top and bottom faces of the unit cell domain for the excitation purpose. Periodic boundary conditions are used to simulate the periodicity of the array structure. In order

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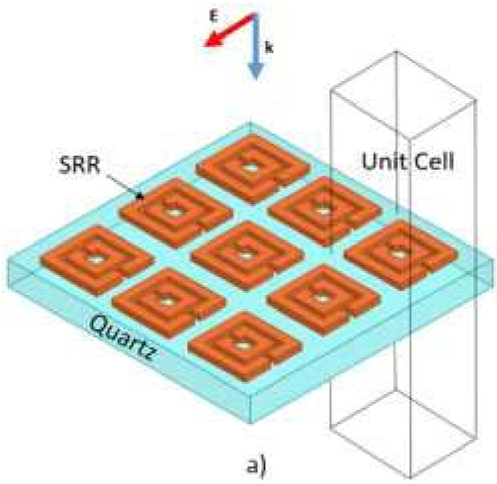

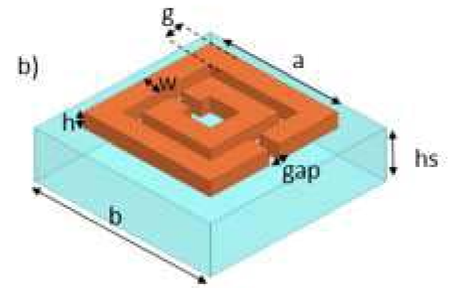

Inputs	a	b	w	h	gap	g	hs
Nominal Values (μm)	26	36	4	3	2	2	10

c)

Fig. 1. (a) Illustration depicting the SRR array on a substrate. (b) Unit cell showing the input parameters. (c) Dimensions of the SRR. The periodic SRR structure is normally illuminated by a plane EM wave.

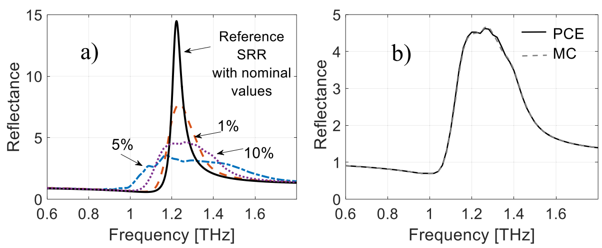

Fig. 2. (a) Computed and estimated reflectance for different uncertainty levels versus frequency. (b) Comparison of the reflectance obtained by PCE and MC techniques for 5% of uncertainty.

to identify the resonance behavior of the SRR at THz frequencies, one calculates the S-parameters corresponding to both transverse electric (TE) and transverse magnetic (TM) modes. The reflectance quantity which is the ratio between the S_{11} parameters of both modes (Reflectance $= S_{11}(\text{TE})/S_{11}(\text{TM})$) is considered. The nominal dimensions for the SRR and the substrate are given in Fig. 1(c).

A. PCE Analysis for the Statistical Reflectance Whose Moments Are Estimated Separately for Each Frequency

In this communication, we considered three levels of uncertainty, 1%, 5%, and 10%. The input parameters are supposed to have uniformly distributed random values around the nominal values given in Fig. 1(c). The accuracy of metamodels constructed using the PCE analysis is assessed by computing the leave one out error between the metamodel and deterministic numerical model outputs and it is found that a few hundreds of data are enough to construct the metamodel and to have the lowest error level.

It should be noted that we constructed a PCE model for each frequency between 0.6 and 1.8 GHz. In other words, randomly selected input parameters data are presented to the deterministic code and the corresponding random output data are calculated separately for each frequency. Thus, due to the operating frequency, the generated set of input–output data has different output data for the same input data. That is said, by means of the constructed PCE metamodels, a mean and a standard deviation of the reflectance are calculated independently at each frequency. Fig. 2(a) shows the reflectance versus the frequency given by HFSS with the nominal values and the estimated average reflectance provided by the PCE models.

The accuracy of the surrogate models can be checked by comparing the PCE and MC outputs. As an example, the average reflectances

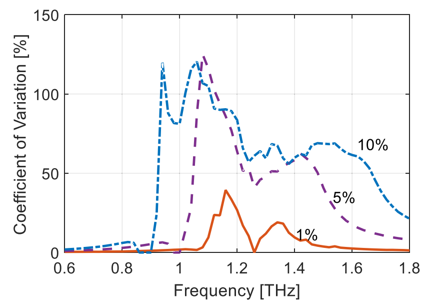

Fig. 3. Coefficient of variation for the three levels of uncertainty on input parameters.

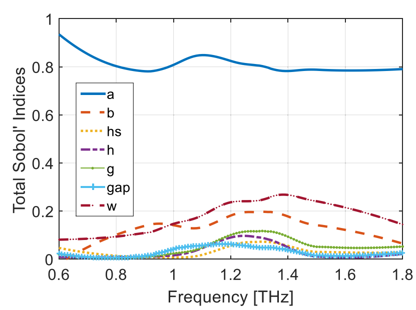

Fig. 4. Sobol' indices versus frequency.

are compared in Fig. 2(b). It is clear from the plots that both outputs have similar behaviors. However, we notice an important distortion of the reflectance around the resonance frequency when the uncertainty becomes higher [Fig. 2(a)]. This fact is confirmed in Fig. 3 where the coefficient of variation (standard deviation/average) $\times$ 100 is plotted.

It can be easily observed that the input parameter having the highest influence on the reflectance is the side length a of the SRR. It has a quasi-stable behavior at all the frequency band. This parameter is followed the wire width w and by the periodicity b of the SRR array which have considerable effect around the resonance. All other parameters have negligible impact.

Finally, the total Sobol' indices that ensure us a good estimation of the importance of each input parameters on the output variance of the physical structure are calculated. The Sobol' indices versus the frequency are presented in Fig. 4.

The dependence of the reflectance on the SRR side length a may be analyzed by keeping in mind that its magnetic resonance is closely

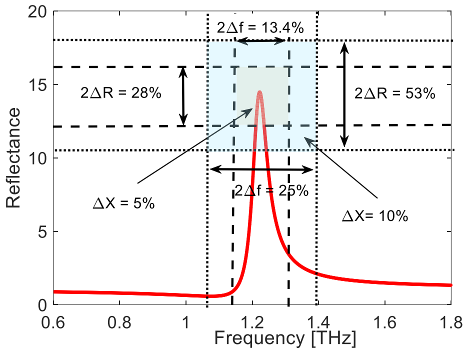

Fig. 5. Schematic displaying the uncertainty of the outputs for two levels of input uncertainty (5% and 10%).

related to the total inductance L given by the combination of the self-inductance of the metallic wire that form the SRR and the mutual inductance formed between the conducting arms of adjacent SRR elements. In fact, the well-known expression $f_r \cong 1/(LC)^{1/2}$ shows that the resonance is inversely proportional to the total inductance. Thus, the variation of the wire length a induces a variation of the inductance which in turn affects the magnetic response of the SRR represented by the reflectance. The longer the wire the higher is the inductance. Similar analysis may be conducted for the width w of the wire. Nevertheless, the inductance L is inversely proportional to the wire width. Therefore, the smaller the width the larger is the inductance. Thus, the resonance should appear at lower frequencies. However, this dependence is weaker compared to the wire length effect. In fact, it has been shown that the inductance is proportional to the area of the SRR which is given mainly by $L \propto a^2$. As for the SRR (metallic wire) height h, the result is as expected, there is no significant influence. Indeed, the height h is much larger than the skin depth at these terahertz frequencies. The variation in the ring separation g and the cuts of the rings gap change the capacitance between the rings and the capacitance formed by the cut of the ring. However, the capacitance has lower effect on the reflectance compared to the inductance. These features have been demonstrated in an earlier work done by Kafesaki *et al.* [16] where left-handed MMs and arrays of SRRs transmission properties have been studied. Especially, it is shown that, the order of the influence of some of the parameters is as follows: $w > g >$ gap $> h$. This order mostly complies with what we obtained from the sensitivity analysis.

B. PCE Analysis of the Resonance Frequency and the Corresponding Amplitude

In Section II-A, we estimated the mean and variance of the reflectance by building a PCE for each frequency. In this part, a different strategy has been adopted to evaluate the uncertainty of the reflectance. Two different outputs have been examined: the resonance frequency and the corresponding reflectance amplitude at the resonance. Thus, for each set of input data, a characteristic reflectance is calculated using the deterministic model, and the resonance frequency and the resonant amplitude are extracted. Thus, two polynomial expansions are dealt with; one for the resonance frequency and another for the amplitude at the resonance. In this section, the same set of input data is used to construct the PCEs. The estimated variations for both random outputs are represented in Fig. 5.

The statistical moments estimated by the PCEs are represented by the colored square area in Fig. 5. The squares are centered at the average values, and the side length of the squares is determined

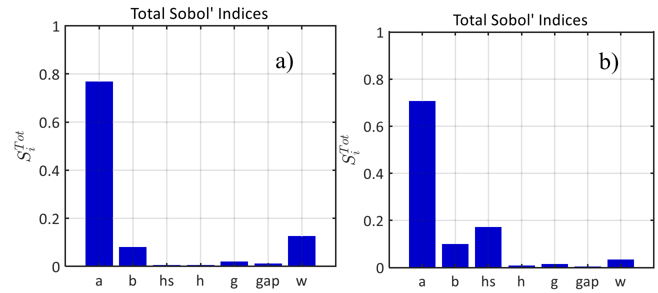

Fig. 6. Sobol' indices indicating the influence of the variation of each input variables to the statistical outputs. (a) Resonance frequency. (b) Amplitude at the resonance.

by calculating the coefficient of variation. Δf is the coefficient of variation of the resonance frequency and ΔR is the coefficient of variation of the amplitude of the reflectance. For example, 10% of variation of the input variables corresponds to 1.25 THz and 14.52 as average values and 12.5% and 26.5% as coefficient of variation of the resonance frequency and amplitude, respectively. As given by the deterministic model, the resonance frequency and the reflectance amplitude corresponding to nominal values (without uncertainty) are 1.22 THz and 14.48, respectively. It can be seen that for both level of uncertainty of the input variables (ΔX), the average values estimated by the PCEs are very close to the deterministic ones. The coefficient of variation can be as high as 12.5% and 26% for the resonance frequency and the amplitude, respectively. The Sobol' indices are estimated according to each PCEs coefficients (Fig. 6).

First, one can notice that the side length a of the SRR has still the largest impact on both outputs. Second, although the other variables have negligible effect on the outputs, there is a considerable change when it comes to the height *hs* of the substrate. In fact, it is seen in Fig. 6 that the height of the substrate has no significant impact on the resonance frequency whereas the amplitude of the reflectance is influenced by it. This behavior is mainly due to the actual nominal thickness of the substrate. In fact, it has been shown in [17] and [18] that the frequency shift is much larger for lower thickness values. Thus, it is expected to have stronger effect of the substrate thickness on the resonance frequency for thinner substrate (hs $\ll 10\ \mu$m).

III. Conclusion

The influence of the uncertainty of the design parameters of an SRR on the reflectance is investigated at terahertz frequencies using the PCE analysis. It has been shown that uncertainties of the design parameters should be considered while designing such a structure. Depending on the uncertainty level of input variables, the resonance frequency may be lost while measuring the reflectance. The amplitude of the reflectance is also highly affected. It appears from our analysis that the most influential parameter in this regard is the side length a of the SRR. The manufacturer of the SRR should be carried out with a special care on this side length. The statistical analysis using the PCE presented in this communication can be applied to any form of MMs to determine the level of uncertainty of the desired output response affected by the variability of the design parameters.

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