Stochastic Collocation based FEM Procedure for Terahertz Structures

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***Abstract*—Small deviations in realized dimensions of THz waveguides may lead to substantial changes in the performance. The geometrical dimensions are assumed to vary randomly with a normal distribution, to represent manufacturing tolerances. In this paper we propose an approach to compute the influence of selected geometric dimensions of a THz corrugated waveguide slow wave structure on its frequency response, phase velocity and the beam voltage. An affine parametric model of the elemental integral equations of the 3D finite element procedure using curl transformations has been used to model the random variations in geometric parameters.**

***Index Terms*—Finite Element Method, Stochastic collocation, Terahertz structures, Geometric tolerance.**

I. Introduction

Practical electromagnetic problems are solved using numerical approaches that strive to approximately satisfy the governing differential equation derived from Maxwell equations. One of the most common and widely used techniques in electromagnetic community is the finite element method (FEM) [1]. Commercial tools like HFSS and COMSOL use an FEM based solver. FEM is a versatile method for modelling interior (closed) domain problems with the complex geometries or inhomogeneously filled geometries.

In many EM problems with complex geometries, one often faces with unexpected variations in material properties and geometric tolerances. Much of these randomness and uncertainty in design parameters of the structure occur due to manufacturing processes. This is especially true for complex geometries at high frequencies, e.g. at THz. With such unavoidable variations, one needs to have a proper statistical model using a stochastic analysis, considering the design parameters as random variables or random fields to match any measurements with simulations.

To demonstrate the utility of the approach, the influence of the uncertain geometric dimensions caused by the fabrication tolerances on critical response parameters of Slow wave structures (SWS), in particular corrugated waveguide TWT structures at THz frequencies has been quantified. SWS are high frequency microwave devices that operate in the GHz to THz frequency range. Depending on the operating frequency, computer numerical controlled (CNC), nano filling, Ultravoilet LIGA, or deep reactive ion etching (DRIE) may be used to fabricate these devices. Fabrication errors due to excessive surface-grinding, residual undercuts and rounded corners causes the change in dimension of the wave guide. This causes the shift in frequency of operation and thus changes the phase velocity and interaction impedance [3]. Accurate knowledge of phase velocity and interaction impedance are very crucial as the small signal gain of the SWS device is sensitive to these parameters [4]. A variation of 0.5% in phase velocity can cause 8 dB change in small signal gain and 10% change in interaction impedance can effect the small signal gain by 5 dB [5]. The study of random fluctuation effects of any of these design parameters using Monte Carlo simulations are not possible due to large computational time of the deterministic solvers. An alternate feasible approach is demonstrated to do the stochastic analysis of large deterministic problems by incorporating the effects of random variations of a geometry into the finite element formulations of electromagnetics.

II. Stochastic Procedure

Consider the generalized matrix eigenvalue equation to be solved with appropriate boundary condition for the dispersion analysis of SWS :

$$\mathbf{A}\,\mathbf{E} = k_0^2\,\mathbf{B}\,\mathbf{E} \tag{1}$$

In a finite element procedure, the local matrix entries corresponding to the edges s, t on an arbitrary element T are given by

$$A_{st} = \int_T \mu_r^{-1}\,(\nabla \times \mathbf{w}_s^*)\,.\,(\nabla \times \mathbf{w}_t^*)\,d\mathbf{x} \tag{2}$$

$$B_{st} = \int_T \epsilon_r\,\mathbf{w}_s\,.\,\mathbf{w}_t\,d\mathbf{x} \tag{3}$$

The above stiffness and mass matrix integrals can be evaluated on the reference element for vector based tetrahedron elements using

$$\begin{aligned} A_{st} &= \int_T \nabla \times \mathbf{w}_s . \nabla \times \mathbf{w}_t\,d\mathbf{x} \\ &= \frac{1}{|\mathbf{J}_T|}\int_T (\mathbf{J}_T\,\nabla \times \hat{\mathbf{w}}_s)\,(\mathbf{J}_T\,\nabla \times \hat{\mathbf{w}}_t)\,d\hat{\mathbf{x}} \end{aligned} \tag{4}$$

$$\begin{aligned} B_{st} &= \int_T \mathbf{w}_s\,.\mathbf{w}_t\,d\mathbf{x} \\ &= |\mathbf{J}_T| \int_{\hat{T}} \left(\mathbf{J}_T^{-T}\,\hat{\mathbf{w}}_s \circ F_T^{-1}\right)^T \left(\mathbf{J}_T^{-T}\,\hat{\mathbf{w}}_s \circ F_T^{-1}\right) d\hat{\mathbf{x}} \end{aligned} \tag{5}$$

where $\mathbf{J}$ is the Jacobian of the transformation of the element T onto a standard reference element $\hat{T}$. The random variation in the geometrical parameters can be simulated by perturbing the finite elements corresponding to the parametric domain.

As a result of the geometric parameter uncertainty, the eigenvalue equation of the system will become random eigenvalue equation of the form

$$\mathbf{A}(\xi)\ \mathbf{E}(\xi) = \lambda(\xi)\ \mathbf{B}(\xi)\ \mathbf{E}(\xi) \tag{6}$$

where $\xi\ (= \xi(\theta))$ is a vector of standard random variables, belongs to the probability space $(\Theta, \mathcal{F}, P)$. The effect of random variations in the geometrical modelling parameter can be taken into account in the finite element matrix constructions by scaling the Jacobians of the local element matrices. This approach can be used to compute the influence of the stochastic variations in geometric dimensions without re-meshing for each perturbation. It maybe noted that conventional FEM procedure, any changes in the model geometry results in changes in the mesh. The above scaling procedure avoids this requirement.

A. Stochastic Collocation

Stochastic collocation is a sampling technique of a random field/variable [5]. The basic principle of stochastic collocation is based on the quadrature sampling of the random space and the functional interpolation of the stochastic response using appropriate basis functions. It is a non-intrusive technique which means that the input to the random system model will be varied but not the actual solution process. The deterministic solvers are used as black boxes for computing the response at collocations points. To compute the stochastic response characteristics, the output response is assumed to have the probability distribution and thus can be expressed in the form of polynomial chaos expansion as

$$f(\xi) = \sum_{k=1}^{M} f_k \Psi_k(\xi) \tag{7}$$

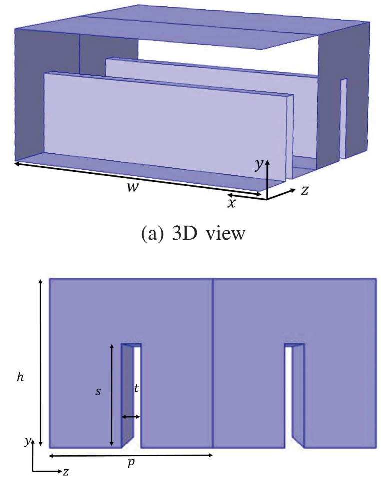
where Ψ_k are appropriate orthogonal polynomials. Lagrange polynomials defined as

$$L_m(\xi)\ =\ \prod_{\substack{j=1\\ j\neq k}}^{m} \frac{(\xi - \xi_j)}{(\xi_k - \xi_j)} \tag{8}$$

such that $L_m(\xi_j) = \delta_{jk}$, m is the number of collocation points, ξ_j is the variable with the node set $\Theta = \{\xi_1 \cdots \xi_m\}$, is often used in interpolation based approach [5], [6]. Once the response of the system f_k is computed using the deterministic solver the statistics and the density function can be evaluated using equation **??**.

B. Monte Carlo Analysis

In the following examples, Monte Carlo simulations are done for validation. The Monte carlo simulation were done for 10^4 trails by running the deterministic solver for each sample from the random vector. The major challenge in Monte carlo simulation is generating a new mesh for each new sample of the random variable. This has been done by changing the coordinates in the .GEO file of the GMSH through MATLAB and there by generating the mesh with new coordinate file.



(a) 3D view

(b) Side View

Fig. 1: Ridged TWT structure

Monte carlo method described in the following steps:
1: Compute N samples of the stochastic variable with given distribution.
2: Solve the deterministic system to obtain the N deterministic solutions.
3: Compute the statistics of the response quantities.
The above Monte Carlo analysis may take several days to arrive at converged solutions. To overcome the unusual computational time and the cost of the Monte carlo analysis, the proposed approach uses the geometric affine element integrals given in Equation **??**.

III. Numerical Example

A. Corrugated Rectangular Waveguide

The corrugated rectangular waveguide structure is a simple structure suitable as slow wave structures at THz frequency range. They are easy to fabricate with the available technologies and simple to assemble [7]. The geometrical dimensions for an SWS operating at 990 GHz are given in Table **??** [8]. Due to the small dimensions of the ridges, especially at the THz frequency range, the geometrical dimensions may vary to the actual design dimensions. Hence the sensitivity analysis of the various design parameters are carried out for a better design and practical specification of the manufacturing tolerance levels. The approach in the above section is used to quantify the influence of geometric variations on the cold test parameters of this TWT structure. The sensitivity analysis is performed on phase velocity, beam voltage and the operational frequency of a SWS.

TABLE I: Design parameters

Geometric parameter	value
w	300 μm
b	130 μm
p	25 μm
s	80 μm
t	15 μm

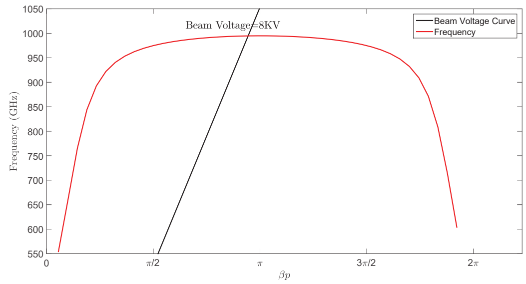


Fig. 2: Dispersion characteristics of the fundamental spatial harmonic

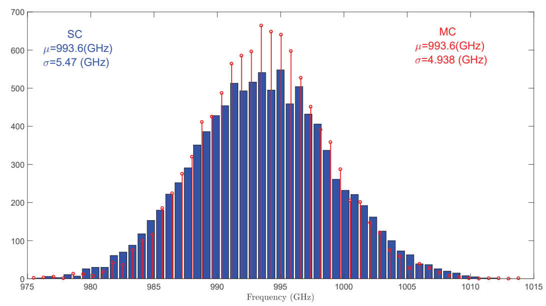


Fig. 3: Frequency Density Function at fixed V_0

The dispersion characteristics for the structure shown in Fig. **??** obtained through deterministic FEM is shown in Fig. **??**. The interaction of the beam voltage curve and the EM wave is found to occur in the fundamental spatial mode. The corresponding beam voltage is obtained from the phase velocity relation is 8 KV.

B. Sensitivity analysis

Sensitivity analysis of the SWS is performed on the phase velocity, beam voltage and frequency of operation using the approach discussed above. We considered 1% change in s, h, w and p, t are assumed to change by ± 0.35 μm. All the parameters are considered to vary as normal distribution. The density plot of the frequency variation obtained using the stochastic collocation approach and Monte Carlo analysis is shown in Fig. **??**. The density functions of the phase velocity and beam voltage curves are shown in Fig. **??** and Fig.**??**.

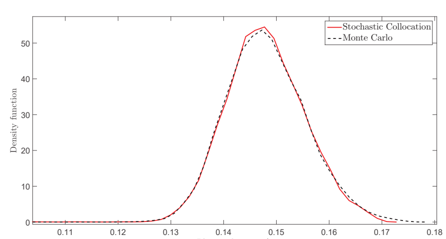


Fig. 4: Phase velocity Density Function at fixed V_0

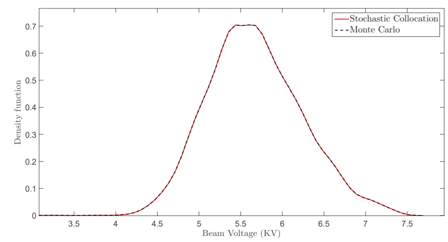


Fig. 5: Ddensity function of Beam Voltage of SWS

IV. Summary

In this paper we demonstrated n approach to incorporate the effects of random variations of a geometry into finite element formulations for electromagnetics. The proposed approach uses the Jacobians of 3D vector FEM formulations to implement the stochastic collocation method for geometric parameters in the problem. The density function for the response characteristics are computed using Lagrange interpolation polynomials.

The cold test characteristics of Slow wave structures at THz frequencies are computed using the finite element method. The sensitivity analysis of phase velocity and the beam voltage characteristics are computed with respect to the geometric parameter variations. The complexity of the solution varies only marginally depending on the number of design variables allowed to have tolerance.

Unlike Mote Carlo approach which requires as many different meshes and repeated simulations as the number of sample variations, the proposed approach is computationally elegant and provides the statistical effects in just one execution.

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