Demystifying Material Parameters for Terahertz Electromagnetic Simulation

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ABSTRACT

Two industry-standard electromagnetic modelling software packages, HFSS™ and CST Microwave Studio®, are used extensively for modelling arbitrary THz structures. However, with both there are a number of practical issues that relate to how such commercially-available software can be used to give results that are meaningful and accurate. In this paper conventional air-filled metal-pipe rectangular waveguides have been simulated, using a raft of different approaches, with a view to illustrating weaknesses in accuracy in a quantifiable way. This paper highlights a number of incorrect approaches, some being intuitive and logical, and makes recommendations for the most appropriate solutions.

INTRODUCTION

With research into terahertz technology receiving increasing attention, commercial electromagnetic (EM) simulation software packages are widely used to predict the performance of THz structures. However, in this frequency range, the frequency dispersion effects in conductivity can affect the results significantly and, therefore, they have to be taken into account when such devices are modelled. Although, commercially-available software packages can generally predict the performance of an arbitrary 3D structure, the correct approach to selecting the most appropriate boundary conditions, defining a material's parameters and entering its real or complex values within the software are not always straightforward. With ambiguous information given in Technical Notes some intuitive and logical approaches also yield incorrect results, which may not be apparent to even experienced EM software users [1, 2].

THz METAL-PIPE RECTANGULAR WAVEGUIDE MODELLING

Metal-pipe rectangular waveguides (MPRWGs) are simulated at THz frequencies, where frequency dispersion in conductivity has previously been found to affect predicted results [2]. Thus, a MPRWG with internal dimensions $a \times b = 100 \times 50\ \mu m^2$ (i.e. JPL-100 standard [2, 6]) with gold walls having room-temperature values $\sigma_o = 4.517 \cdot 10^7$ S/m, $\tau = 27.135$ fs and μ_r = 0.99996 was used as the reference structure. To simplify the analysis, the waveguide is assumed to operate in the fundamental TE_{10} mode, so that closed-form analytical expression for the propagation constant can be used [5] for direct comparison with the simulated results.

Now, in HFSS™ [3], the classical skin-effect model is employed by default, with the bulk dc conductivity σ_o being entered in the material setup dialog box. Alternatively, the simple relaxation-effect model can be used by entering a data file containing the non-complex (i.e. real) only conductivity values calculated *a priori* at each discrete frequency point. These two models can be used either as boundary conditions or as intrinsic 'solid object' material parameters, with the results reported for the latter approach being used without meshing inside the metal objects. It must be noted, however, that the classical relaxation-effect model cannot be used directly; while existing versions of HFSS™ allow complex numbers to be entered into the conductivity value field it does not actually support these complex values [2], as will be explained here in greater detail.

For example, with the Finite Conductivity Boundary (FCB), complex conductivity values can be entered using the following syntaxes: $\sigma' \pm \sigma"j$ or $\sigma' \pm \sigma"i$. Here, the imaginary term $\sigma"$ is simply ignored in calculations, thus giving results that coincide with the simple relaxation-effect model [2]. Alternatively, complex conductivity values can be entered using the following syntax [7]: *cmplx*(σ', σ''), where $\sigma'' \geq 0$ only. Unfortunately, it has been found that this latter method gives incorrect results. The problems associated with the FCB are also the same for the Layered Impedance Boundary (LIB), since both boundaries use the conductivity value σ as the input parameter. However, with the Impedance Boundary (IB), the appropriate complex surface impedance Z_s can be entered directly for each discrete frequency point. In this case, the results reported by HFSS™ are in excellent agreement with the analytical model [2]. It

must be noted, however, that since the complex value of surface impedance must be entered *a priori*, significant errors may result if tuning or optimization routines are employed with structures where the spectral feature(s) of interest can shift to frequencies not represented by the list of discrete frequency points that characterise the surface impedance.

The above approaches are also valid in CST Microwave Studio® (CST MWS) [4], where the classical skin-effect and simple relaxation-effect models can be obtained using either the conducting wall boundary (CWB) or the intrinsic bulk conductivity. However, with the simple relaxation-effect model, the conductivity values have to be entered at each discrete frequency point, since the software does not currently support a data file import for conductivity. Again, the classical relaxation-effect model cannot be used explicitly, but the "surface impedance" material (SIM) type can be defined with a data file containing the complex surface impedance values at each discrete frequency point. Fortunately, CST MWS interpolates between data points and thus tuning or optimization routines can be employed, in contrast to HFSS™. Although, the results increasingly diverge from the analytical model as frequency increases; the reason for this is unknown. Alternatively, an "ohmic sheet" material type can be used where the surface impedance is defined at each discrete frequency point. Unfortunately, this approach is impractical because a very dense mesh is needed in order to get accurate results. Also, in principle, the solid walls of the waveguide can be treated as dielectrics (i.e. a "normal" material type) by defining the angular plasma frequency ω_p and collision damping angular frequency $\omega_\tau = 1/\tau$ of the metal, but it has also been found that the results are incorrect.

CONCLUSION

In this paper, various approaches to modelling simple geometry THz metal structures, employing frequency dispersive metals, have been studied and the most suitable approach indicated. Since defining a material's parameters and entering its real and/or complex values within the software are not always straightforward, choosing the wrong approach may yield incorrect results. Thus, this paper has explained in detail how to properly define a material's parameters and choose the most appropriate boundary condition in order that a THz structure can be modelled with meaningful results.

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