Invited Paper

Engineering Approach to Modelling Metal THz Structures

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Abstract: When compared to the over-simplified classical skin-effect model, the accurate classical relaxation-effect modelling approach for THz structures at room temperature can be mathematically cumbersome and not insightful. This paper briefly introduces various interrelated electrical engineering concepts as tools for characterizing the intrinsic frequency dispersive nature of normal metals at room temperature. This engineering approach dramatically simplifies the otherwise complex analysis and allows for a much deeper insight to be gained into the classical relaxation-effect model. Three example applications are given for the calculation of important parameters and associated errors with hollow metal-pipe rectangular waveguides (MPRWGs), hollow MPRWG cavity resonators and single metal planar shield.

Keywords: Engineering approach, terahertz dispersion, metals

1. Introduction

Some well-known commercial electromagnetic modelling software packages currently employ over-simplified frequency dispersion models for the conductivity of metals used to predict the performance of THz structures at room temperature. For example, Ansoft's High Frequency Structure Simulator (HFSS™) is considered by some to represent a benchmark standard in electromagnetic modelling software, even though it can give anomalous results under certain conditions (e.g., electrically thin-walled MPRWGs [1] and THz MPRWG structures [2]).

The MPRWG represents one of the most important forms of guided-wave structure for terahertz applications. Well-known commercial electromagnetic modelling software packages currently employ over-simplified intrinsic frequency dispersion models for the bulk conductivity of normal metals used in terahertz structures at room temperature. Various conductivity modelling strategies for normal metals at room temperature have previously been compared for characterizing rectangular waveguides and associated cavity resonators between 0.9 and 12 *THz* [2]. A quantitative analysis for the application of different models used to describe the intrinsic frequency dispersion nature of bulk conductivity at room temperature was undertaken [2]. When compared to the use of the accurate relaxation-effect model, it was found that HFSS™ (Versions 10 and 11) gives a default error in the attenuation constant for MPRWGs of 108% at 12 *THz* and 41% errors in both Q-factor and overall frequency detuning with a 7.3 *THz* cavity resonator. With the former, measured transmission losses are significantly lower than those predicted using the current version of HFSS™, which may lead to an underestimate of THz losses attributed to extrinsic effects. With the latter error, in overall frequency detuning, the measured positions of return loss zeros, within a multi-pole filter, will not be accurately predicted by HFSS™. For this reason, calculating the errors that result from using the over-simplified classical skin-effect frequency dispersion model for normal metals at room temperature is important at THz frequencies.

The use of the accurate classical relaxation-effect model for frequency dispersion in normal metals at room temperature with THz structures can be mathematically cumbersome and not insightful. The recent introduction of the Engineering Approach [3-5] demonstrated that it is possible to dramatically simplify otherwise complex analysis and allows for a much deeper insight to be gained into the classical relaxation-effect model. Here, the interrelated concepts of equivalent transmission line modelling, kinetic inductance modelling, Q-factor modelling and complex skin depth modelling are all introduced for the characterization of normal metals at room temperature for applications in THz structures [3]. For example, using the concept of Q-factor, the synthesized equivalent transmission line model was validated for a metal [4]. Then, using the concept of complex skin depth, analysis was performed on hollow MPRWGs and their associated cavity resonators [4]. This work proved that the mathematical modelling of THz structures can be greatly simplified by taking an electrical engineering approach to these electromagnetic problems.

The engineering approach was then applied to investigate room temperature THz metal shielding [5]. It was shown that, with the simplest case of a uniform plane wave at normal incidence to an infinite single planar shield in air, all figure of merit parameters for the shield can be accurately characterized. The errors introduced by adopting the traditional and much simpler classical skin-effect model were also quantified. In addition, errors resulting from adopting well-established approximations have also been investigated and quantified. It was shown that the engineering approach allows analytical expressions to be greatly simplified and predictive equivalent transmission line models to be synthesized, to give a much deeper insight into the behavior of room temperature THz metal shielding. For example, it is shown that figures of merit and associated errors (resulting from the use of different classical frequency dispersion models) become essentially thickness invariant when the physical thickness of the shield is greater than 3 normal skin depths.

2. THz Metal-Pipe Rectangular Waveguide Modelling

Fig. 1 shows a uniform hollow MPRWG defined within the Cartesian coordinate system *xyz*. Transmission is along the *z* direction, and over a distance *d*, with internal cross-sectional dimensions *a* and *b*. The structure in Fig. 1 has the ideal (i.e. lossless) dominant-mode guided wavelength given by the following textbook expression [15]:

$$\lambda_{g\_ideal} = \frac{\lambda_o}{\sqrt{1-\left(\frac{\lambda_o}{\lambda_c}\right)^2}} = \frac{\lambda_o}{\sqrt{1-\left(\frac{f_c}{f}\right)^2}} \quad (1)$$

where, λ_o is the free space wavelength; $\lambda_c = 2a$ is the ideal cut-off wavelength; *a* is the internal width dimension of the MPRWG; $f_c = c/2a$ is the ideal cut-off frequency for the dominant TE_{10} mode; and *c* is the speed of light in free space.

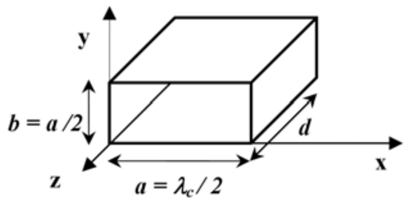


Fig. 1 Internal spatial variable definitions for a uniform hollow MPRWG [2].

The attenuation constant for this guided-wave structure can be obtained directly from the real part of the propagation constant, i.e. $\alpha = \Re\{\gamma_{mo}\}$. For the dominant TE_{10} mode, the following expressions for attenuation constant can be calculated, based on the intrinsic frequency dispersion models for normal metals at room temperature. For the classical relaxation-effect model, variables are indicated by the suffix "*R*"; for the simple relaxation-effect model, variables are indicated by the suffix "*R'* "; and for the classical skin-effect model, variables are indicated by the suffix "*o*".

Classical relaxation-effect model   Simple relaxation-effect model   Classical skin-effect model

$$\alpha_R = \Re\{\gamma_{10R}\};\ \gamma_{10R} = f\{Z_{SR}\} \qquad \alpha_{R'} = \Re\{\gamma_{10R'}\};\ \gamma_{10R'} = f\{Z_{SR'}\} \qquad \alpha_o = \Re\{\gamma_{10o}\};\ \gamma_{10o} = f\{Z_{So}\} \quad (2)$$

Using (2) with the simple *Power Loss* approximation method [2], for calculating attenuation constant in terms of the real part of the surface impedance only, it is easy to calculate the percentage error in attenuation constant for the simple relaxation-effect model $E_{\alpha_{R'}}$ and classical skin-effect model E_{α_o}, relative to the classical relaxation-effect model:

$$E_{\alpha_{R'}} = \left(\frac{\alpha_{R'} - \alpha_R}{\alpha_R}\right)\cdot 100\ \% \cong \left[\sqrt{\frac{1+(\omega\tau)^2}{\sqrt{1+(\omega\tau)^2} - \omega\tau}} - 1\right]\cdot 100\ \%$$

$$E_{\alpha_o} = \left(\frac{\alpha_o - \alpha_R}{\alpha_R}\right)\cdot 100\,\% \cong \left[\sqrt{\sqrt{1+(\omega\tau)^2} + \omega\tau} - 1\right]\cdot 100\,\% \qquad (3)$$

Here, angular frequency $\omega = 2\pi f$, where f is the frequency of the driving electromagnetic fields, and the phenomenological temperature-dependent scattering relaxation time for the free electrons (i.e. mean time between collisions) τ in normal metals at room temperature.

For simplicity, it will be assumed throughout that the MPRWGs will have a height dimension of $b = a/2$. The attenuation constants and resulting errors have been plotted against frequency, and are shown in Fig. 2. To a first degree of approximation, it can be seen that the error increases linearly with frequency for the classical skin-effect model; with a 108% error at 12 *THz*. The error obtained with the simple relaxation-effect model is 373% at 12 *THz*.

The engineering approach gives the following expressions:

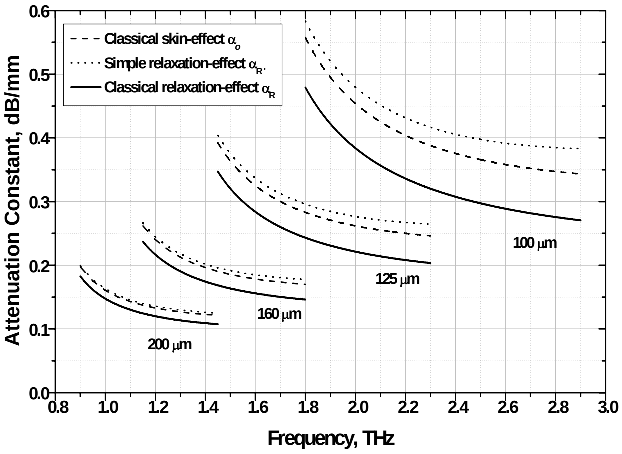
$$Q_{cR} = \frac{\Re\{\gamma_R\}}{\Im\{\gamma_R\}} = (1 + \xi\, Q_{mR})^2 \qquad (4)$$

where $\xi = \sqrt{\sqrt{u^{-4} + u^{-2}} + u^{-1}} - u^{-1}$ and $Q_{mR} = \dfrac{\Re\{\gamma_R^2\}}{\Im\{\gamma_R^2\}} = \omega\tau = u$

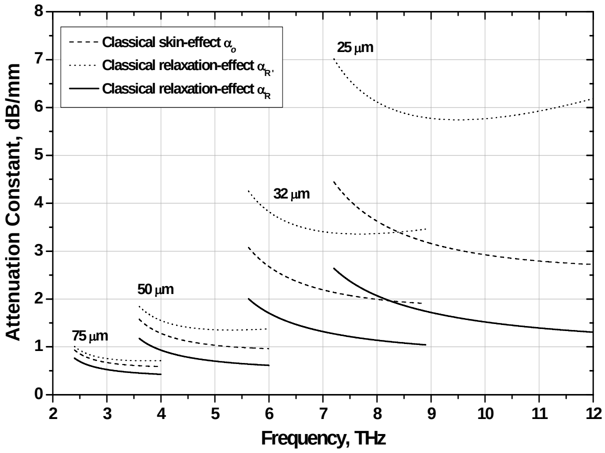
where Q_{cR} and Q_{mR} are the component and material Q-factors, respectively, for a normal metal [3]. Now, $\xi = f(\omega\tau)$ was found empirically to approximate a constant value of 0.539, resulting in a worst-case error of only 0.96% from dc to $\omega\tau$ = 2. As a result, an expression for the error in attenuation constant when using the classical skin-effect model can be greatly simplified to the following [4]:

$$E_{\alpha_o}(\omega) = \left(\sqrt{Q_{cR}} - 1\right)\cdot 100\% = \xi Q_{mR} \cdot 100\% \approx 0.539 Q_{mR} \cdot 100\% \quad \text{for} \quad 0 \le \omega\tau \le 2 \tag{5}$$

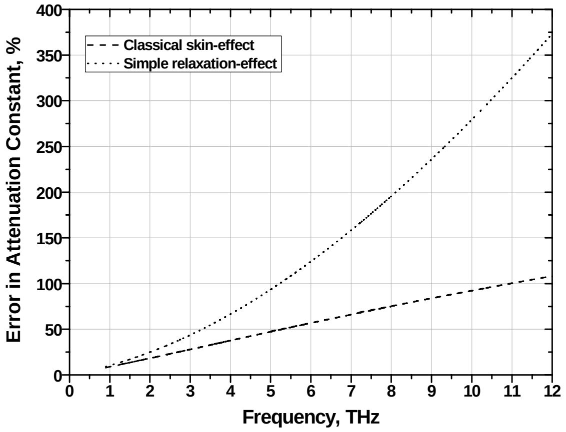
Using (5), the calculated error using this simple approximation is 110% at 12 *THz* (i.e. at $\omega\tau = 2.046$) and this can be compared with the exact calculated error, using (3), of 108% at the same frequency [4].



(a)



(b)

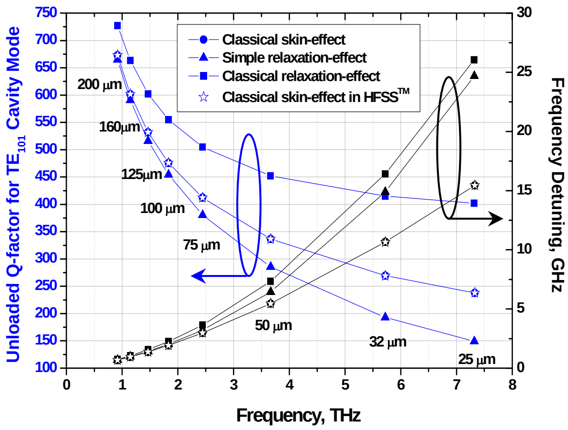


(c)

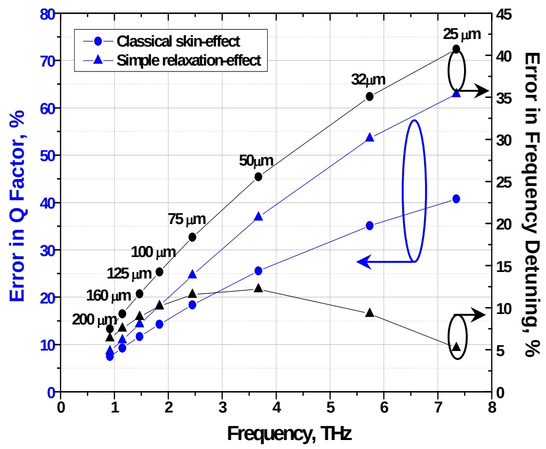
Fig. 2 Calculated attenuation constants for the dominant TE_{10} mode: (a) JPL bands; (b) our bands; and (c) resulting errors in attenuation constants [2].

3. THz Cavity Resonator Modelling

For a hollow half-height MPRWG cavity resonator with $d = \sqrt{2}a$, the calculated and HFSS™ simulated values for unloaded Q-factor and overall frequency detuning are plotted in Fig. 3(a), for the dominant TE_{101} mode [2]. The resulting errors in unloaded Q-factor and overall frequency detuning, relative to the classical relaxation-effect model, are given in Fig. 3(b) and show an almost identical frequency response for both with the classical skin-effect model. Here, a 41% error is calculated for a 7.3 *THz* cavity resonator. A much lower error is found in the overall frequency detuning with the simple relaxation-effect model; with a worst-case value of 12% for a 3.7 *THz* cavity resonator. However, a 63% error in the unloaded Q-factor has been calculated with the simple relaxation-effect model for a 7.3 *THz* cavity resonator.



(a)



(b)

Fig. 3 (a) Unloaded Q-factor and overall frequency detuning for TE_{101} cavity mode, at the resonant frequencies; and (b) resulting errors in Q factors and frequency detuning [2].

With the unloaded Q-factor calculated using the over-simplified classical skin-effect model the resulting error, relative to the values calculated using the classical relaxation-effect model, was previously determined after undergoing a relatively lengthy process [2]. However, in contrast, a relatively simple expression for this error is derived using the concept of Q-factor for normal metals at room temperature [4]:

$$E_{Qo}(\omega'_{oR}) = \left|\frac{Q_{Uo}(\omega'_{oo}) - Q_{UR}(\omega'_{oR})}{Q_{UR}(\omega'_{oR})}\right| \times 100\,\% = \left|\sqrt{\frac{Q_{mR}(\omega'_{oR})}{Q_{mR}(\omega'_{oo})Q_{cR}(\omega'_{oR})}} - 1\right| \times 100\,\% \tag{6}$$

$$E_{Qo}(\omega'_{oR}) \cong \left|\frac{1}{\sqrt{Q_{cR}(\omega'_{oR})}} - 1\right| \times 100\,\% \qquad \text{since} \qquad \omega'_{oR} \cong \omega'_{oo} \tag{7}$$

$$\therefore E_{Qo}(\omega'_{oR}) \approx \left(\frac{1}{1 + 1.8553\, Q_{mR}(\omega'_{oR})^{-1}}\right) \times 100\,\% \qquad \text{for} \qquad 0 \le \omega\tau \le 2 \tag{8}$$

For example, using (8), the calculated error using this simple approximation is 40% at 7.3 *THz* (i.e. at $\omega\tau = 1.245$) and this can be compared with the exact error determined using the lengthy technique described in [2] of 41% at the same frequency.

4. THz Single Metal Planar Shield

For simplicity, an infinite single metal planar shield in air will be considered, with uniform plane wave at normal incidence, as illustrated in Fig. 4.

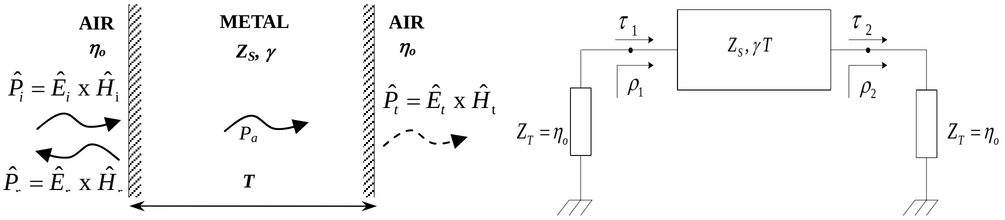


Fig. 4 Uniform plane wave at normal incidence to an infinite single metal planar shield in air: (a) physical representation; and (b) equivalent 2-port network model [5].

For the analysis of a single metal planar shield, an addition to the engineering approach was the introduction of the boundary resistance coefficient $k = \frac{\eta_o}{R_S} >> Q_c \ge 1$, where k represents the ratio of intrinsic impedance of free space to the surface resistance of the metal. Moreover, it is useful to represent the physical thickness T of the metal shield in terms of the number a of normal skin depths $\delta_S = 1/\alpha$ (i.e. $T \to a\,\delta_S$). Thus, it can be easily shown that the exponential decay for the intensity of the electromagnetic fields within the metal can be represented by the following exponent [5]:

$$-\gamma T \to -\gamma \cdot a\,\delta_S = -a \cdot \left(1 + \frac{j}{Q_c}\right) \tag{9}$$

Using the classical relaxation-effect model to describe frequency dispersion within a normal metal at room temperature, $T = a_R\,\delta_{SR}$. Also, for the classical skin-effect model:

$$a_o = \frac{T}{\delta_{So}} = a_R \left(\frac{\delta_{SR}}{\delta_{So}}\right) \tag{10}$$

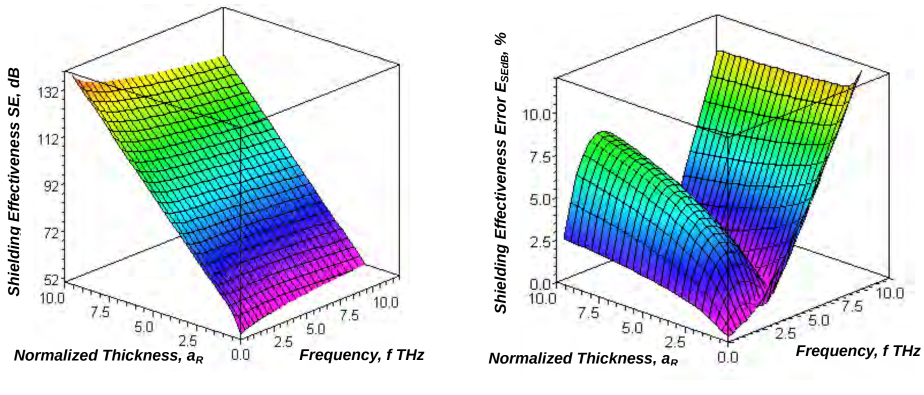
The transmission power isolation that results from a shield can be defined by its shielding effectiveness (SE). Using the exact expressions given [5], the overall shielding effectiveness has been calculated for gold at room temperature using the classical relaxation-effect model. The results are represented by the contour plot shown in Fig. 5(a). The results from Fig. 5(a) can be compared with those calculated using the classical skin-effect model (more traditionally associated with screening effectiveness calculations) using the following expression for the resulting error in shielding effectiveness E_{SE}:

$$E_{SE\,dB} = \left|\frac{SE_{dBo} - SE_{dBR}}{SE_{dBR}}\right| \cdot 100\% \tag{11}$$

where SE_{dBR} and SE_{dBo} are the screening effectiveness calculated using the classical relaxation-effect and skin-effect models, respectively. Using the engineering approach, it can be shown the following more elegant expressions can be given for these figures of merit parameters, without introducing errors greater than 0.1% [5]:

$$SE_{dBR} \cong 10\log_{10}\left(\frac{8\left(1+Q_{cR}^2\right)/k_R^2}{\cosh(2a_R) - \cos(2a_R/Q_{cR})}\right) \quad \text{and} \quad SE_{dBo} \cong 10\log_{10}\left(\frac{16/k_o^2}{\cosh(2a_o) - \cos(2a_o)}\right) \tag{12}$$

The shielding effectiveness error results are represented by the contour plot shown in Fig. 5(b).



(a) (b)

Fig. 5 Screening effectiveness calculations: (a) using classical relaxation-effect model; (b) resulting error when compared to classical skin-effect model calculations [5].

5. Conclusion

The engineering approach was developed for accurately modelling intrinsic frequency dispersion within a metal. For example, it can explain how wavelength can increase proportionally with frequency at higher terahertz frequencies [3].Using the engineering approach, THz metal-pipe rectangular waveguides, associated cavity resonators and single metal planar shields have been accurately characterized and errors that result from the use of the over-simplified skin-effect model for describing the frequency dispersion within normal metals at room temperature have been calculated. It should be noted that the analysis given here is only a small representation of that covered in the cited papers from the same authors of this paper.

While the focus has been on the characterization of normal metals (magnetic and non-magnetic) at room temperature, it is believed that the same methodology may be applied to metals operating in anomalous frequency-temperature regions, superconductors, semiconductors, carbon nanotubes and metamaterials.

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