THz Applications for the Engineering Approach to Modelling Frequency Dispersion within Normal Metals at Room Temperature

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Abstract— 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. Recent work has 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. This paper gives applications for this engineering approach. Here, using the concept of Q-factor for a metal, the synthesized equivalent transmission line model is validated. Then, using the concept of complex skin depth, analysis is performed on hollow metal-pipe rectangular waveguides and their associated cavity resonators. This work proves that the mathematical modelling of THz structures can be greatly simplified by taking an electrical engineering approach to these electromagnetic problems.

1. INTRODUCTION

The classical relaxation-effect model accurately describes the frequency dispersive nature of normal metals at room temperature. Indeed, the robustness of this model has been tested in recent years for normal metals at room temperature from dc to terahertz frequencies [1–4]. For example, it has been used to validate measurements [1], alternative frequency dispersion models [2, 3] and commercial electromagnetic simulation software [4]. However, when compared to the over-simplified classical skin-effect model (with associated variables indicated by the suffix "o"), the classical relaxation-effect modelling approach (with associated variables indicated by the suffix "R") for THz structures at room temperature can be mathematically cumbersome and not insightful.

Given an 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, a recent paper addressed analysis for all values of $\omega \tau$ and even allowed accurate simplifying assumptions to be made in the region of $0 \le \omega \tau \le 2$. In this paper, the equivalent transmission line model is tested and metal-pipe rectangular waveguide structures are modelled [4] using the concepts of Q-factors and complex skin depth for normal metals at room temperature [5].

2. EQUIVALENT TRANSMISSION LINE MODEL VALIDATION

The modelling of frequency dispersion in a metal using a synthesized equivalent transmission line model has been recently reported but not extensively validated [5]. Therefore, the modelling of an electromagnetic wave travelling to an arbitrary depth of one wavelength will be modelled here using ABCD parameter matrices and its results converted into S-parameters for comparison.

For a uniform passive transmission line, the ABCD parameter matrix is given by the following textbook representation:

$$[ABCD] = \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} \cosh(\gamma l) & Zo\sinh(\gamma l) \\ Yo\sinh(\gamma l) & \cosh(\gamma l) \end{bmatrix} \qquad Yo = \frac{1}{Zo} [S] \tag{1}$$

where, for any arbitrary uniform transmission line, γ is the complex propagation constant, l is the physical length and Zo is the complex characteristic impedance. For the equivalent transmission line model, the characteristic impedance equates to the surface impedance of the metal, i.e., $Zo = Z_S$, when the electromagnetic waves decay exponentially with distance into the metal (as found with normal metals at room temperature) [5]. The corresponding S-parameters are given by the following textbook representation:

$$S_{11} = S_{22} = \frac{(Z_T - Z_T^*)\cosh(\gamma l) + (Zo - Z_T^* Z_T Yo)\sinh(\gamma l)}{D}$$
(2)

$$S_{21} = S_{12} = \frac{2R_T}{D}$$

$$D = 2Z_T \cosh(\gamma l) + (Zo + Z_T^2 Yo) \sinh(\gamma l) [\Omega]$$

$$Z_T = R_T + jX_T [\Omega] \text{ and } Z_T^* = R_T - jX_T [\Omega]$$

where Z_T is the complex terminating impedance at both ends of the transmission line and $j = \sqrt{-1}$ is the complex operator. When the terminating impedance is equal to the complex conjugate of the characteristic impedance of the transmission line (i.e., $Z_T = Zo^*$):

$$S_{11} = S_{22} = \frac{-je^{-2\gamma l}Q_c(1+jQ_c)}{1+(e^{-\gamma l}Q_c)^2} \cong -je^{-2\gamma l}Q_c(1+jQ_c) \quad \text{with} \quad \Re\{\gamma\}l > 2.3$$

$$S_{21} = S_{12} = \frac{e^{-\gamma l}(1+jQ_c)}{1+(e^{-\gamma l}Q_c)^2} \cong e^{-\gamma l}(1+jQ_c) \quad \text{with} \quad \Re\{\gamma\}l > 2.3$$

Insertion Loss = 20 log|s₂₁| [dB] $\Rightarrow G_{\text{MAX}}$ [dB]
(3)

Attenuation = $20 \log(\Re\{s_{21}\})$ [dB] \Rightarrow Absoption Loss = $20 \log(e^{-\Re\{\gamma\}l})$ [dB]

where Q_c is the component Q-factor for a normal metal [5]. For a depth of one wavelength (i.e., $l = \lambda$), with the classical relaxation-effect model, the propagation constant per unit wavelength and voltage-wave transmission coefficients $S_{21} = S_{12}$ are given by the following simple expressions:

$$\gamma_R \lambda_R = 2\pi \frac{\gamma_R}{\Im\{\gamma_R\}} = 2\pi (Q_{CR} + j) \left[\lambda_R^{-1}\right]$$

$$S_{11} = S_{22} \cong 0 \quad \text{and} \quad S_{21} = S_{12} \cong e^{-2\pi Q_{cR}} \left(1 + jQ_{cR}\right)$$

$$(4)$$

 $Q_{cR} = \frac{\Re\{\gamma_R\}}{\Im\{\gamma_R\}} = (1 + \xi Q_{mR})^2$ where $\xi = \sqrt{\sqrt{u^{-4} + u^{-2}} + u^{-1}} - u^{-1}$ and $Q_{mR} = \frac{\Re\{\gamma_R^2\}}{\Im\{\gamma_R^2\}} = \omega \tau = u$ where Q_{cR} and Q_{mR} are the component and material Q-factors, respectively, for a normal metal using the classical relaxation-effect model [5].

The equivalent transmission line model for the classical relaxation-effect model is shown in Fig. 1. The corresponding ABCD parameter matrix for the elementary lumped-element circuit is given in (5):

$$[ABCD_{1}] = \begin{bmatrix} A_{1} & B_{1} \\ C_{1} & D_{1} \end{bmatrix} = \begin{bmatrix} 1 + j\omega\mu\sigma_{R}\Delta z^{2} & j\omega\mu\Delta z \\ \sigma_{R}\Delta z & 1 \end{bmatrix}$$

$$\Delta z = \frac{\lambda_{R}}{N} = \frac{\pi\delta_{So}}{N}Q_{cR}^{3/2} \left[1 + \frac{1}{Q_{cR}^{2}} \right]$$
(5)

where $\mu = \mu_o \mu_r$ is the magnetic permeability, μ_o is the magnetic permeability of free space, μ_r is the relative magnetic permeability, $\sigma_R = \sigma_o/(1 + j\omega\tau)$ is the intrinsic bulk conductivity due to free charge carriers, $\Delta z = f(\omega\tau)$ represents the propagation distance for one elementary lumpedelement circuit (this must be very much shorter than the wavelength λ of the electromagnetic wave within the metal), δ_{So} is the normal skin depth calculated using the classical skin-effect model and N is the number of cascaded elementary lumped-element circuit sections.



Figure 1: Equivalent transmission line model for the classical relaxation-effect model, showing expressions for the distributed-element parameters [5].



Figure 2: Frequency responses for the forward voltage-wave transmission coefficient for gold at room temperature, for N = 800 sections.

For the synthesized equivalent transmission line model, the overall ABCD parameter matrix can be calculated from:

$$[ABCD_N] = \prod_{i=1}^{N} [ABCD_1(i)] \tag{6}$$

A good test for the validity of the equivalent transmission line model, for both the reflection and transmission characteristics, is to extract the surface impedance $Z_{SR}|_N$ and propagation constant per unit wavelength $\gamma_R \lambda_R|_N$, respectively, from the overall *ABCD* parameter matrix [*ABCD*_N]:

$$Z_{SR}|_{N} = \sqrt{\frac{B_{N}}{C_{N}}} \quad \text{and} \quad \gamma_{R}\lambda_{R}|_{N} = \cosh^{-1}(A_{N}) = \sinh^{-1}\left(\frac{B_{N}}{Z_{SR}|_{N}}\right) \tag{7}$$

The results from theory, using (1) to (4), can be compared with those from the corresponding synthesized equivalent transmission line model, extracted using commercial circuit simulation software (Agilent Technologies EEsof ADS), for gold at room temperature (having $\sigma_o = 4.517 \times 10^7 \,[\text{S/m}]$, $\tau = 27.135 \,[\text{fs}]$, $\mu_r = 0.99996 \cong 1 \,[1]$). Fig. 2 shows the frequency responses for the forward voltage-wave transmission coefficient. It can be clearly seen that there is an excellent fit between theory and that from the equivalent transmission line model having N = 800 sections.

It is interesting to note that the phase angle for S_{21} increases with frequency, unlike a normal transmission line. As a result, the differential-phase group delay will be negative. However, this does not break the laws of physics, since the transit time propagation delay is still positive.

A more detailed comparison between theory, using (1) to (4), results from the ABCD parameter matrix calculation, using (5) to (7), and commercial circuit simulation software (Microwave Office(R)) is given in Table 1, for an arbitrary frequency of $\omega \tau = 1$, i.e., $f = 1/(2\pi\tau) = 5.865$ THz.

The reason for choosing this frequency is for mathematical simplicity, since $Q_{cR}(\omega\tau = 1) = (1 + \sqrt{2})$ [5]; hence, the propagation constant per unit wavelength simplifies to:

$$\gamma_R \lambda_R(\omega \tau = 1) = 2\pi \left[\left(1 + \sqrt{2} \right) + j \right] \left[\lambda_R^{-1} \right] \tag{8}$$

The results of the test in (7) can be seen in Table 1, for N = 400 and 800. It can be seen that the reflection characteristic is identical to the theoretical value, to 8 decimal places, with 800 sections. However, the transmission characteristic is only determined to 3 decimal places, with 800 sections. Note that an extracted value of $\Im\{\gamma_R\}\lambda_R = 0$ gives the same answer as the theoretical value of 2π . With regard to the S-parameters and their associated power characteristics, it can be seen in Table 1 that there is an excellent agreement between the results from the commercial circuit simulation software and the ABCD parameter matrix calculations. Also, the results are closer to the corresponding theoretical values as the number of sections increase from 400 to 800.

Parameters for $l = \lambda_R, \ \omega \tau = 1, \ Z_T = Z_{SR}^*$	Theory	Synthesized Transmission Line			
		ABCD Parameter		Microwave Office®	
		Matrix Calculations			
No. of Sections, N		400	800	400	800
$Z_{SR}\left[\Omega ight]$	0.46079043	0.46079964	0.46079043		
	+j1.11244650	+j1.11246875	+j1.11244650		
$\gamma_R\lambda_R[\lambda_R^{-1}]$	15.1689	15.1681	15.1685		
	+j6.2832	-j0.0013	-j0.0004		
\mathbf{S}_{11}	0	0.0006	0.0002	0.0006	0.0001
		+j0.0271	+j0.0135	+j0.0270	+j0.0133
Return Loss [dB]	-247.51	-31.35	-37.41	-31.37	-36.9
$S_{21} = e^{-2\pi(1+\sqrt{2})}$	2.583	2.579	2.582	2.564	2.567
$\cdot [1+j(1+\sqrt{2})] \times 10^7$	+j6.237	+j6.242	+j6.240	+j6.238	+j6.239
${ m G}_{MAX}\left[{ m dB} ight]$	-123.4126	-123.4093	-123.4099	-123.41	-123.4
Attenuation Loss [dB]	-131.756	-131.748	-131.752	-131.9	-131.9
$\forall S_{21} = \tan^{-1}(1+\sqrt{2}) [\circ]$	67.50	67.55	67.52	67.58	67.56

Table 1: Comparison of modelled parameters for gold at room temperature, at 5.865 THz, determined from theory, direct ABCD parameter matrix calculations and synthesized equivalent transmission line models using commercial circuit simulation software.

3. MODELLING OF WAVEGUIDE STRCTURES AT ROOM TEMPERATURE

Equations for the surface impedance of a metal, the attenuation constant of uniform metal-pipe rectangular waveguides (MPRWGs) and the Q-factor of resonant waveguide cavities were previously given for accurate calculations at THz frequencies [4].

3.1. Metal-pipe Rectagular Waveguides

With hollow metal-pipe rectangular waveguides operating in the dominant TE₁₀ mode of propagation, above its cut-off angular frequency $\omega_c|_{TE_{10}}$, the attenuation constant attributed to the finite conductivity of the metal walls is given by the well-known textbook expression:

$$\alpha_{WG}|_{\mathrm{TE}_{10}} = \frac{Rs(\omega)}{\eta_o} G_{10}(\omega) \left[\mathrm{Np/m}\right] \tag{9}$$

$$Zs(\omega) = \sqrt{\frac{j\omega\mu_o\mu_r}{\sigma + j\omega\varepsilon_o}} \left[\Omega/\text{square}\right]; \quad \eta_o = \sqrt{\frac{\mu_o}{\varepsilon_o}} \left[\Omega\right]; \quad G_{10}(\omega) = \frac{1 + 2\frac{b}{a} \left(\frac{\omega_c|_{\text{TE}_{10}}}{\omega}\right)^2}{b\sqrt{1 - \left(\frac{\omega_c|_{\text{TE}_{10}}}{\omega}\right)^2}} \left[\text{m}^{-1}\right] (10)$$

where $Zs(\omega) = Rs(\omega) + jXs(\omega)$ is the surface impedance of the metal, $R_S = \Re\{Z_S\}$ is the surface resistance, $X_S = \Im\{Z_S\}$ is the surface reactance, η_o is the intrinsic impedance for a plane wave in free space, ε_o is the electric permittivity of free space, $\sigma \equiv \sigma' - j\sigma''$ is the intrinsic bulk conductivity of the metal due to free charge carriers, and $G_{10}(\omega)$ is the geometric factor for the TE₁₀ mode with this particular structure. With reference to Fig. 3, the internal width and height dimensions are *a* and *b*, respectively.

Now, the attenuation constant for this uniform guided-wave structure can be calculated using the over-simplified classical skin-effect model. Using this approach the resulting errors, relative to the values calculated using the classical relaxation-effect model, were previously determined by the following complicated expression [4].

$$E_{\alpha_o}(\omega) = \left(\frac{\alpha_{WGo} - \alpha_{WGR}}{\alpha_{WGR}}\right) \cdot 100\% \cong \left[\sqrt{\sqrt{1 + (\omega\tau)^2} + \omega\tau} - 1\right] \cdot 100\% \ [4] \tag{11}$$

However, in contrast, a relatively simple expression for this error can now be derived using the

concept of Q-factor for normal metals at room temperature [5]:

$$E_{\alpha_o}(\omega) \cong \left(\frac{R_{So} - R_{SR}}{R_{SR}}\right) \cdot 100\% \quad \text{with} \quad Z_{SR} = R_{So} \left[\frac{1}{(1 + \xi\omega\tau)} + j\left(1 + \xi\omega\tau\right)\right] \tag{12}$$

$$\therefore E_{\alpha_o}(\omega) = \left(\sqrt{Q_{cR}} - 1\right) \cdot 100\% = \xi Q_{mR} \cdot 100\% \approx 0.539 Q_{mR} \cdot 100\% \quad \text{for} \quad 0 \le \omega\tau \le 2 \ [5]$$
(13)

For example, using (13), 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 calculated error, using (11), of 108% at the same frequency.

3.2. Cavity Resonators

The unloaded Q-factor for a hollow metal-pipe rectangular waveguide cavity resonator in the mnl mode is given as:

$$Q_U\left(\omega_o'\right)\big|_{\mathrm{TE}_{mnl}} = \frac{\omega_{I_mnl}}{R_S\left(\omega_o'\right)}\Gamma_{mnl} \tag{14}$$

where ω_{I_mnl} is the ideal angular resonant frequency for the TE_{mnl} modes in an ideal (lossless) hollow cavity and $R_S(\omega'_o)$ is the surface resistance of the metal walls at the angular resonant frequency ω'_o . Here, overall frequency detuning of ω'_o from ω_{I_mnl} is because of both perturbation and frequency detuning due to ohmic losses [4]. The corresponding geometric factor Γ_{mnl} for this particular resonant cavity structure is given by:

$$\Gamma_{mnl} = \mu_o \psi_{mnl} [H] \quad \text{where} \quad \psi_{mnl} = \frac{\lambda_{I_mnl}}{8} \left[\frac{2b \left(a^2 + d^2\right)^{3/2}}{2b \left(a^3 + d^3\right) + ad \left(a^2 + d^2\right)} \right] \text{ [m]} \tag{15}$$

where d is the internal length dimension for the cavity resonator. The corresponding textbook expression for the wavelength in free space λ_{I_mnl} at the associated resonant frequencies for the TE_{mnl} modes in an ideal hollow cavity f_{I_mnl} is give by:

$$\lambda_{I_mnl} = \frac{c}{f_{I_mnl}} \quad \text{where} \quad f_{I_mnl} = \frac{c}{2} \sqrt{\left(\frac{m}{a}\right)^2 + \left(\frac{n}{b}\right)^2 + \left(\frac{l}{d}\right)^2} \equiv \frac{\omega_{I_mnl}}{2\pi} \tag{16}$$

where c is the speed of light in free space. For example, with the dominant TE_{101} mode, it can be seen that (15) and (16) reduce to:

$$\lambda_{I_101} = \frac{2ad}{\sqrt{a^2 + d^2}} = \begin{cases} \sqrt{2}a & \text{for } b = a/2 & \text{and } d = a \ [5] \\ \sqrt{8/3}a & \text{for } b = a/2 & \text{and } d = \sqrt{2}a \ [4] \end{cases}$$
(17)

$$\psi_{101} = \frac{abd(a^2 + d^2)}{2[2b(a^3 + d^3) + ad(a^2 + d^2)]} = \begin{cases} \text{Volume/Area for } d = a \ [5] \\ a/8 \text{ for } b = a/2 \text{ and } d = a \\ 3a/[2(\sqrt{2} + 10)] \text{ for } b = a/2 \text{ and } d = \sqrt{2}a \ [4] \end{cases}$$
(18)

With the classical skin-effect model, it will be seen that the surface resistance is given by the textbook expression:

$$R_S(\omega'_o) \to R_{So}(\omega'_{oo}) = \frac{\omega'_{oo}\mu_o\mu_r\delta_{So}(\omega'_{oo})}{2}$$
(19)



Figure 3: Internal spatial variable definitions for a uniform hollow MPRWG.

The resulting unloaded Q-factor is, therefore, given as:

$$Q_{Uo}(\omega_{oo}')\big|_{\mathrm{TE}_{mnl}} = \frac{2}{\mu_r \delta_{So}(\omega_{oo}')} \left(\frac{\omega_{I_mnl}}{\omega_{oo}'}\right) \psi_{mnl}$$
(20)

With the classical relaxation-effect model, it has recently been shown in [5] that the surface resistance becomes:

$$R_S(\omega'_o) \to R_{SR}(\omega'_{oR}) = \omega'_{oR}\mu_o\mu_r\Im\left\{\delta_{cR}(\omega'_{oR})\right\}$$
(21)

where complex skin depth is given by $\delta_{cR} \equiv \delta'_{cR} - j\delta''_{cR}$ [5]. The resulting unloaded Q-factor is, therefore, now given by the following:

$$Q_{UR}\left(\omega_{oR}'\right)\Big|_{\mathrm{TE}_{mnl}} = \frac{1}{\mu_r \Im\left\{\delta_{cR}\left(\omega_{oR}'\right)\right\}} \left(\frac{\omega_{I_mnl}}{\omega_{oR}'}\right) \psi_{mnl}$$
(22)

Note that (22) represents the formal derivation of $Q_U(\omega'_o)$ in [4], for a hollow rectangular waveguide cavity having metal walls with $\mu_r \neq 1$ and $\omega \tau > 0$; this is also the more general form of $Q_{UR}(\omega_{oR})|_{TE_{101}}$ in [5].

It is interesting to see how the unloaded Q-factor for this component can be represented using the exact expression from the classical skin-effect model (20) at $\omega \tau = 1$, by including both component and material Q-factors for the normal metal walls:

$$Q_{Uo}\left(\omega_{oo}^{\prime}\right)\big|_{\mathrm{TE}_{mnl}} = \frac{Q_{Uo}\left(\omega\tau=1\right)\big|_{\mathrm{TE}_{mnl}}}{\sqrt{Q_{mR}\left(\omega_{oo}^{\prime}\right)}} \text{ and } Q_{UR}\left(\omega_{oR}^{\prime}\right)\big|_{\mathrm{TE}_{mnl}} = Q_{Uo}\left(\omega\tau=1\right)\big|_{\mathrm{TE}_{mnl}}\sqrt{\frac{Q_{cR}\left(\omega_{oR}^{\prime}\right)}{Q_{mR}\left(\omega_{oR}^{\prime}\right)}}$$
(23)

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 [4]. However, in contrast, a relatively simple expression for this error can now be derived using the concept of Q-factor for normal metals at room temperature:

$$E_{Qo}(\omega'_{oR}) = \left| \frac{Q_{Uo}(\omega'_{oo}) - Q_{UR}(\omega'_{oR})}{Q_{UR}(\omega'_{oR})} \right| \cdot 100\% = \left| \sqrt{\frac{Q_{mR}(\omega'_{oR})}{Q_{mR}(\omega'_{oo})Q_{cR}(\omega'_{oR})}} - 1 \right| \cdot 100\%$$
(24)

$$E_{Qo}\left(\omega_{oR}'\right) \cong \left|\frac{1}{\sqrt{Q_{cR}\left(\omega_{oR}'\right)}} - 1\right| \cdot 100\% \quad \text{since} \quad \omega_{oR}' \cong \omega_{oo}' \tag{25}$$

$$\therefore E_{Qo}\left(\omega_{oR}'\right) \approx \left(\frac{1}{1+1.8553Q_{mR}\left(\omega_{oR}'\right)^{-1}}\right) \cdot 100\% \quad \text{for} \quad 0 \le \omega\tau \le 2 \ [5]$$

$$(26)$$

For example, using (26), 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 error determined using the lengthy technique, described in [4], of 41% at the same frequency.

4. CONCLUSION

This paper has validated the recently introduced engineering approach to modelling frequency dispersion in normal metals at room temperature. While relatively simple examples were previously given, to show how algebraic expressions can be dramatically simplified [5], similar benefits have been demonstrated here with more complicated analytical problems. Using the concept of Q-factor for a metal, the equivalent transmission line model was validated. Then, using the concept of complex skin depth, analysis was performed on hollow metal-pipe rectangular waveguides and their associated cavity resonators. This work proves that the mathematical modelling of THz structures can be greatly simplified by taking an electrical engineering approach to these electromagnetic problems.

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