Error Analysis of Model-Based Frequency- and Time-Domain Methods for THz Material Parameter Extraction

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Abstract— **We investigate quantitatively the error of physical material-model based schemes for time-domain and frequency-domain analyses used to extract material-parameters from measurements acquired by THz time-domain spectroscopy (TDS) systems. An analytic analysis of the noise induced error and its effect on both methods is presented. Especially critical cases with strong resonance features and limited signal-to-noise ratio are addressed.**

I. INTRODUCTION

ONE very active field in THz research and development is the spectroscopic investigation of materials for characterization and recognition purposes. Many substances of interest, like explosives, drugs, pharmaceuticals and chemicals, show unique spectral characteristics in this range [1-2]. By deriving material parameters like the complex refractive index, the complex dielectric constant or related properties, those characteristics can be evaluated [3-4]. One robust approach to determine such parameters from experiments measurements is the combination of a common, single frequency step propagation formalism with a model based analysis. This analysis determines the material parameters by utilizing a mathematical description of their underlying physical processes valid over the complete spectral range [5]. Due to the resulting complete description of the samples transfer function, these analyses can not only be performed in frequency-domain (FD) but are also enabled in time-domain (TD).

The comparison of the results of a time-domain approach and a corresponding frequency-domain method applied to simulated, noisy datasets, which allow fully controllable, independent testing-scenarios, show strong differences between both methods with regard to the overall quality of the extracted data and robustness to noise-induced-errors, especially at strong spectral features. Here we provide a formal investigation of the performance of these approaches especially in the context of quantifying noise effects on parameter extraction procedures. The findings are complemented by an equivalent evaluation of measured, experimental data.

II. RESULTS

The simulated dataset utilized for the performance comparison were acquired by generating a replica transient, resembling the form of an actual TDS system. This transient was on the one hand used as the reference transient of the parameter determination process and on the other hand provides the sample transient by convolution with a modelled sample transfer function. To evaluate the robustness of both concepts, noise of various levels was added to this transient pair. The error of the extracted parameters in reference to the designed ones is determined as a measure of quality.

Fig. 1 depicts the spectral signal-to-noise ratio (SNR) of the investigated sample datasets labeled with the comparison of the resulting mean squared error (MSE) of the extracted material parameters determined by TD and FD methods. The TD approach shows an overall better performance for high SNRs and also maintains an about 10^3 times lower MSE in scenarios of a SNR close or at 0 dB at positions of the spectral features. The TD method even enables an extraction of parameters with a low error rate in cases where multiple spectral features drop below the noise floor. These situations are usually a limitation for classical extraction schemes, restricting the utilizable spectral range to obtain a samples parameters [6].

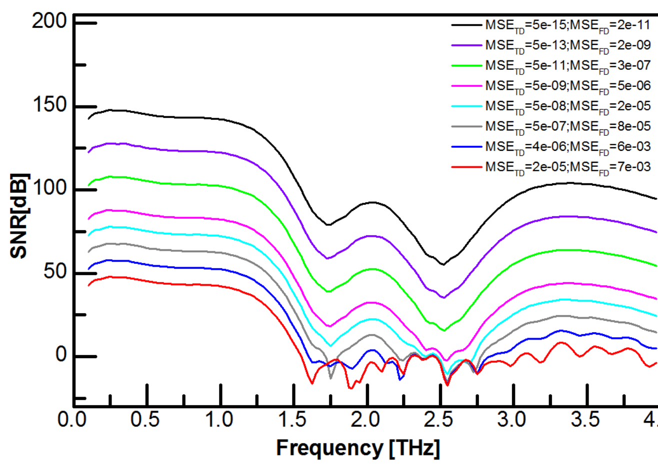

Fig. 1. Spectral SNR of the investigated datasets. The labels show the resulting MSE of the extracted material parameters using TD and FD methods.

In order to determine the cause for the performance differences of both concepts the influence of the initial noise and its level on the different processing stages has to be determined, especially focusing on the steps used exclusively in one of the methods. Following the formalisms for the propagation of noise from TD into FD derived in [7] and [8], the standard deviation (STD) and variance (VAR) of the spectral magnitude and phase data can be expressed as a function of the Fourier transform and STD of the respective input transients.

Fig. 2 accordingly shows the standard deviations of the spectral phase-information (σ_{arg}), derived from the noisy transient-data, labeled with the MSE in correspondence to Fig. 1. It can be seen, that the STD, which is a direct measure of the error, peaks at the positions were the SNR is reduced due to the spectral absorption features, reaching values larger π and is also raised at the neighboring frequencies. The STD further increases drastically with the reduction of the overall

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SNR. Therefore the phase values of the features, represented as turning or saddle points of the phase, are especially disturbed, which results in an erroneous phase-unwrapping, due to the exceedance of the unambiguity threshold of -π/π of the unwrapping procedures. As a consequence actual, feature induced, large phase changes are falsely removed or an artificial jump is inserted. Since the unwrapping introduces a dependency of neighboring phase-points, these errors propagate to the unwrapped phase-values at higher frequency, causing an offset of a complete section of the evaluated spectral phase. These large scale deviations cannot be compensated by the use of the material model in FD and thereby a proper parameter extraction, also at the frequency range unaffected by the offset, is inhibited. The TD processing, in contrast to FD, does not require a phase-unwrapping procedure and is thereby not restricted by this effect, limiting the influence of the spectrally localized increase of noise-induced error on the overall parameter extraction. The determination and evaluation of the phase STD is therefore a valuable tool to assess absolute limits for the applicability of FD methods to the analysis of noisy THz transient data.

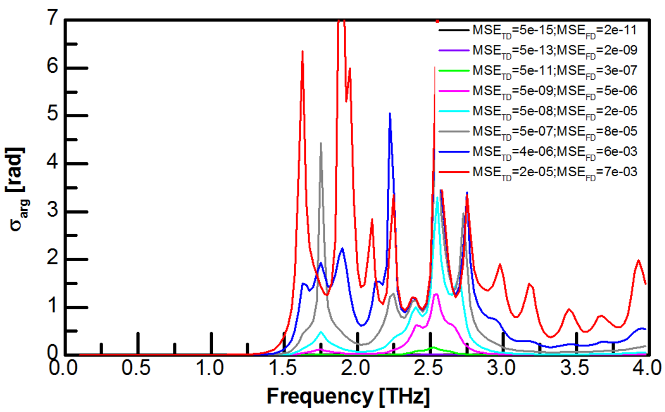

Fig. 2. Standard deviation σ_{arg} of the spectral phase-information, corresponding to datasets of Fig. 1, labeled with the resulting MSE.

III. SUMMARY

We quantitatively investigated the error in material-parameters determined by physical material-model based TD and FD based extraction concepts. A comparison based on simulated noisy data-sets showed an overall lower MSE of the time-domain method at low noise scenarios. Furthermore especially at situations of an SNR of the spectral feature close to 0 dB the TD approach outperformed its FD counterpart by an about 10^3 times lower MSE. The cause for the difference in performance of both concepts could be determined by investigating the transfer of noise, respectively the standard deviation of the transients, form TD into FD. Especially focusing on the standard deviation of the phase, its drastic increase at positions of resonant absorption features could be noted. Considering the requirement of phase-unwrapping of the FD method, these increases in phase-error inhibited the proper operation of the unwrapping procedures, resulting in an offset of phase-data and consequentially the failure of the FD parameter extraction. Since the TD concept does not require an unwrapping it stayed unaffected. The standard deviation phase hence provided the capability to determine the boundaries of FD processing concepts in the presence of noise.

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