Comparison of Model-Based Material Parameter Extraction in Frequency- and Time-Domain

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***Abstract*—We compare physical material-model based schemes for time-domain and frequency-domain analysis of measurement data. Such approaches can be used to extract material-parameters from measurements acquired by THz time-domain spectroscopy (TDS) systems. A detailed intercomparison of both analytic methods is presented. Cases with resonance features and limited dynamic range are considered.**

I. INTRODUCTION

THE spectroscopic investigation of materials for characterization and recognition is a very active field in THz research and development, since many interesting substance (e.g. explosives, drugs, pharmaceuticals, chemicals) show unique spectral characteristics in this range [1]. To evaluate those characteristics, material parameters independent of sample dimensions and measurement system, like the complex refractive index or complex dielectric constant, have to be reliably derived from the measured spectral data. Common approaches to extract material parameters, like a sequential, single frequency step difference minimization method [2] are quite sensitive to the noise at the individual frequencies and translate this noise to the extracted parameters. A more robust concept is the use of a model based analysis that utilizes a mathematical description of the physical processes, like the Lorentz oscillator model, that determine the respective material parameters valid over the complete spectral range [3]. These analyses can be performed in frequency-domain or, with a suitable transformation, in time-domain.

Here we compare a time-domain approach (Fig. 1) to a corresponding frequency-domain method (Fig. 2). By applying both schemes to simulated, noisy datasets we can create reproducible testing-scenarios with full control over spectral features and experimental conditions, independently from the properties of a measurement system. This also simplifies the evaluation of causes for the different performances of the concepts. We complement our investigation by applying both methods also to measured, experimental data, which will be shown during the presentation.

II. RESULTS

Fig. 1 und Fig. 2 depict the extracted refractive indices of both approaches in comparison to the original input refractive index as a function of varying noise/dynamic range (DR) in the transients. The corresponding extinction-coefficients are not shown here, though they confirm the following observations as the behavior is analogous and the numerical extraction of the refractive index is more sensitive to low signal to noise data. It can be seen that the time-domain analysis reaches the ideal fit at a 10 time higher noise level (DR=10^4) compared to the frequency-domain approach (DR=10^5). Even for higher noise levels, the refractive index extracted by the time-domain approach show better agreement to the original refractive index up to a DR of only 10^2. This demonstrates a clear advantage of time-domain based analytic procedures compared to frequency-domain based methods. This difference follows from the phase ambiguity of frequency-based approaches. The time-domain analysis does not rely on unwrapped phase-data and is hence not affected by this inadequacy.

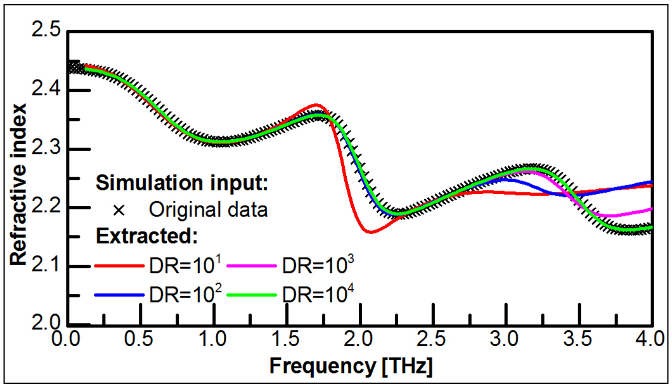

Fig. 1. Refractive index extracted by time-domain analysis of simulated, noisy data. The results for different, decreasing noise levels (increasing dynamic range (DR)) are compared to the original input refractive index (black x) of the simulation.

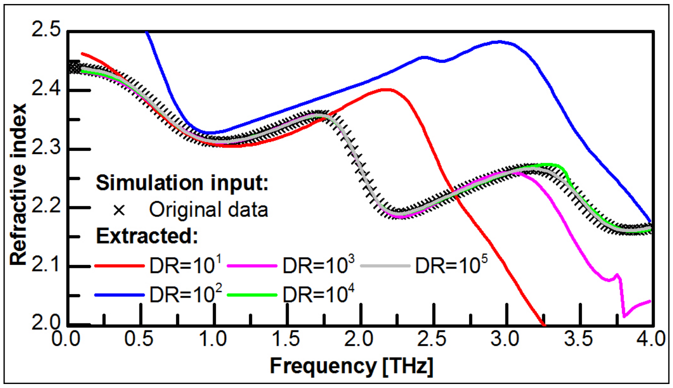

Fig. 2. Refractive index extracted by frequency-domain analysis of simulated, noisy data. The results for different, decreasing noise levels (increasing dynamic range (DR)) are compared to the original input refractive index (black x) of the simulation. The input phase data has been offset-corrected.

Fig. 3 and Fig.4 show the extracted refractive index for a material with strong resonant absorption features for the time-domain and frequency-domain methods respectively, compared to the original indices. It can be seen, that the time-domain approach provides similar results in regards to noise sensitivity, compared to the previous simulation, while the frequency-domain approach doesn't reach a correct result even for the noise-free case (DR=10$^{\infty}$). It is clearly recognizable that the strong feature at 0.8THz is not reconstructed correctly, especially the steep change of the index between the two turning points. This failure of the frequency-domain approach again arises from its stringent requirement for correctly unwrapped phase-information. The large phase-changes at strong features exceed the phase-unambiguity limit of the phase-unwrapping which leads to faulty phase-data and thereby to an erroneous parameter determination. Consequently the sensitivity to phase-errors not only limits the use of frequency-domain approaches for noisy measurement situations, but also affects its applicability for investigations of materials with strong spectral features.

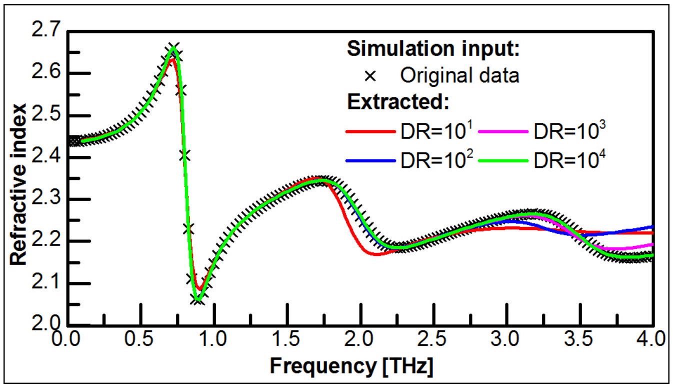

Fig. 3. Refractive index extracted by time-domain analysis of simulated, noisy data with a strong spectral feature. The results for different, decreasing noise levels (increasing dynamic range (DR)) are compared to the original input refractive index (black x) of the simulation.

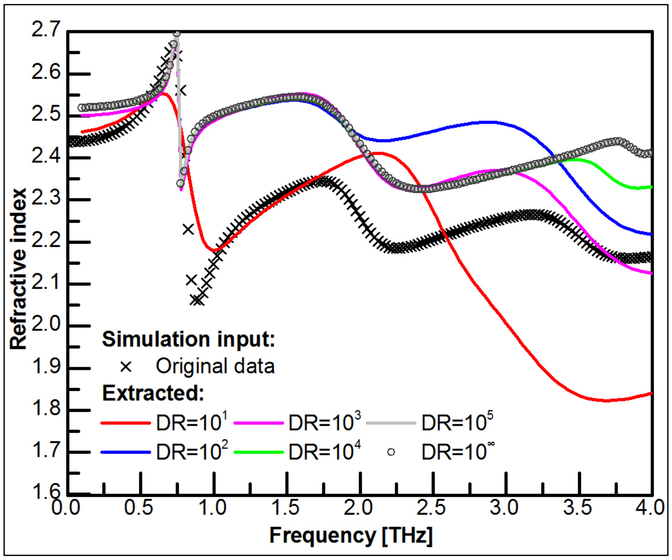

Fig. 4. Refractive index extracted by frequency-domain analysis of simulated, noisy data with a strong spectral feature. The results for different, decreasing noise levels (increasing dynamic range (DR)) are compared to the original input refractive index (black x) of the simulation. The input phase data has been offset-corrected.

III. SUMMARY

We have compared the effects of noise and strong spectral features on the performance of model-based material parameter extraction schemes in frequency- and time-domain. By applying these methods on simulated, noisy datasets we have shown, that the time-domain approach reaches a match to the original input-refractive index at a 10 time higher noise level compared to the frequency-domain analysis and also exhibits superior agreement for higher noise-levels up to a DR of 102. Furthermore we have demonstrated that a large phase change due to a strong spectral feature can inhibit a correct extraction by the frequency-domain method even in a noise-free case, while the time-domain scheme is unaffected.

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