A maximum-likelihood analysis framework for terahertz time-domain spectroscopy

J. Steven Dodge*†, Laleh Mohtashemi*, Paul Westlund*, Payam Mousavi*, Derek G. Sahota*
*Department of Physics, Simon Fraser University, Canada
†Canadian Institute for Advanced Research, Toronto, ON, Canada
Email: jsdodge@sfu.ca

***Abstract*—We present a maximum-likelihood framework for analyzing terahertz time-domain spectroscopy measurements. This approach has several advantages other commonly-used methods, especially for evaluating goodness of fit. We also demonstrate a simple time-domain noise model that accurately describes the noise amplitude in a set of repeated measurements. These techniques are broadly applicable to material parameter estimation.**

I. Introduction and Background

While terahertz time-domain spectroscopy (THz-TDS) measurements are performed in the time domain, they typically are represented and analyzed in the frequency domain using standard signal processing techniques [1], [2]. But since the measurement noise is also structured in the time domain, the transformation to the frequency domain can produce artifacts that can render the results difficult to interpret [3]. We describe a maximum-likelihood (ML) approach to THz-TDS analysis that addresses this weakness. We treat both the signal and the noise explicitly in the time domain, but we constrain the frequency-domain relationship between the input signal and the output signal. We discuss the advantages of this approach.

II. Results

Figure 1 shows the results of a simplified analysis for illustration. Fig. 1(a) shows fifty THz-TDS waveforms, which we assume are noisy measurements of an unknown, band-limited signal $\mu(t)$ subject to both amplitude drift and temporal drift, so that the underlying signal associated with each measurement j is $\zeta(t;A_j,\eta_j) = A_j\mu(t-\eta_j)$. We further assume that the measurements $x_{ij} = x_j(t_i)$ of the underlying waveforms $\zeta_{ij} = \zeta(t_i;A_j,\eta_j)$ include additive, multiplicative, and timebase noise. A ML analysis of this model yields the total noise amplitude $\sigma(t)$ shown in Fig. 1(b), which shows good agreement with the measured time-domain noise obtained from Fig. 1(a). Figure 1(c) shows the normalized residuals $(x-\zeta)/\sigma$, which demonstrates consistency with the randomness assumptions of the ML framework.

We have extended this analysis to determine the basic parameters that determine the Drude conductivity in metals and the electrodynamics properties of superconductors. We find that the ML framework provides consistently more reliable results than the conventional frequency-domain analysis. Moreover, we have found that standard statistical methods, such as the χ^2 test, provide reliable guidance for assessing goodness-of-fit within our framework, while conventional frequency-domain analysis suffers from several inconsistencies in its underlying assumptions.

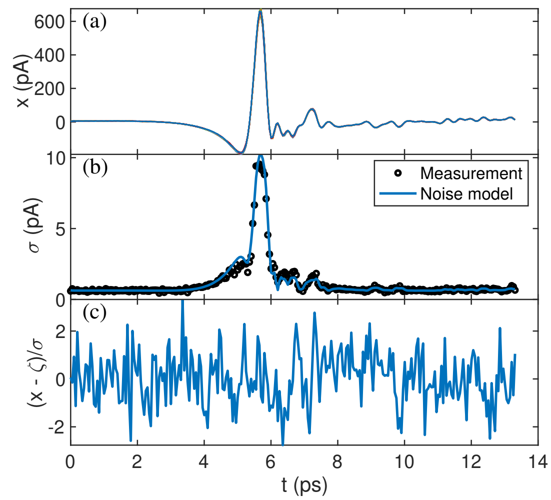

Fig. 1. (a) A set of fifty THz-TDS measurements $X(t)$. (b) Measured time-domain noise amplitude compared to the noise model obtained with the ML method. (c) Residuals of one THz-TDS measurement with respect to the waveform $\zeta(t)$ determined from the ML method, normalized to the noise model shown in (b). The normalized residual distribution is consistent with a gaussian.

III. Conclusion

The ML framework improves on existing methods for THz-TDS in several ways. It can account more readily for the observed noise structure in THz-TDS measurements, it offers standard statistical tests for evaluating the quality of the fit, and it offers more reliable measurements of material parameters.

References

[1] L. Duvillaret, F. Garet, and J.-L. Coutaz, "Highly precise determination of optical constants and sample thickness in terahertz time-domain spectroscopy," Appl. Opt. **38**, 409 (1999).
[2] T. D. Dorney, R. G. Baraniuk, and D. M. Mittleman, "Material parameter estimation with terahertz time-domain spectroscopy," J. Opt. Soc. Am. A **18**, 1562–1571 (2001).
[3] M. Naftaly, R. G. Clarke, D. A. Humphreys, and N. M. Ridler, "Metrology state-of-the-art and challenges in broadband phase-sensitive terahertz measurements," Proc. IEEE **105**, 1151–1165 (2017).