











THzTools: data analysis software for terahertz time-domain spectroscopy

Jonathan Posada Loaiza ^{1*}, Santiago Higuera-Quintero ^{1*}, Alireza Noori ^{1*}, Laleh Mohtashemi ^{1*}, R. P. Hall ¹, Naod Ayalew Yimam ¹, and J. Steven Dodge ^{1¶}

¹ Department of Physics, Simon Fraser University, Canada ¶ Corresponding author * These authors contributed equally.

DOI: [10.21105/joss.07542](https://doi.org/10.21105/joss.07542)

Software

- [Review](#) 
- [Repository](#) 
- [Archive](#) 

Editor: [Chris Vernon](#)  

Reviewers:

- [@crvernon](#)

Submitted: 23 November 2024

Published: 02 December 2024

License

Authors of papers retain copyright and release the work under a Creative Commons Attribution 4.0 International License ([CC BY 4.0](#)).

Summary

Terahertz time-domain spectroscopy (THz-TDS) uses short electromagnetic pulses to probe the electromagnetic response of matter over frequencies from about 0.1 THz to about 10 THz, where $1 \text{ THz} = 10^{12} \text{ Hz}$ (Neu & Schmuttenmaer, 2018). A typical measurement compares two electromagnetic pulses, one of which has interacted with a material and another which has not. The pulses are measured as a function of time, but the electromagnetic properties of matter are most naturally described as a function of frequency, so statistical signal processing techniques must be used to relate the time-domain measurements to the frequency-domain properties of interest. The THzTools package provides an interface for implementing maximum-likelihood methods for THz-TDS analysis, described previously (Mohtashemi et al., 2021).

Statement of need

In the conventional approach to THz-TDS analysis (Neu & Schmuttenmaer, 2018), one transforms the time-domain measurements into the frequency domain for further analysis. This approach has well-known problems, however, which can be resolved by using a maximum-likelihood estimation procedure in the time domain (Mohtashemi et al., 2021). To support this mode of analysis, the THzTools package provides functionality and documentation that are unavailable in existing THz-TDS analysis software (Lee et al., 2023; Peretti et al., 2019; Tayvab et al., 2021). It provides functions to simulate THz-TDS measurements, apply a frequency response function to a THz-TDS waveform, characterize the noise of a THz-TDS system, and fit a parameterized frequency response function to a pair of input and output waveforms.

We developed some of the functionality of THzTools in an earlier MATLAB implementation, which remains undocumented (Dodge et al., 2021). After translating this codebase to Python, we introduced new functionality, optimized the code for speed and efficiency, and revised the user interface to make it easier to use.

Acknowledgements

J. P. L. and S. H.-G. acknowledge support from Mitacs Globalink Research Internship Program. A. N. acknowledges support from the Natural Sciences and Engineering Research Council of Canada Collaborative Research and Training Experience (NSERC CREATE) Program in Quantum Computing. J. S. D. acknowledges support from the Natural Sciences and Engineering Research Council of Canada (NSERC).

References

- Dodge, J. S., Mohtashemi, L., Westlund, P., Sahota, D. G., Lea, G. B., Bushfield, I., & Mousavi, P. (2021). *MATLAB functions for maximum-likelihood parameter estimation in terahertz time-domain spectroscopy*. Zenodo. <https://doi.org/10.5281/zenodo.4326594>
- Lee, J., Leung, C. K., Ma, M., Ward-Berry, J., Santitewagun, S., & Zeitler, J. A. (2023). The dotTHz Project: A Standard Data Format for Terahertz Time-Domain Data. *Journal of Infrared, Millimeter, and Terahertz Waves*, 44(11), 795–813. <https://doi.org/10.1007/s10762-023-00947-w>
- Mohtashemi, L., Westlund, P., Sahota, D. G., Lea, G. B., Bushfield, I., Mousavi, P., & Dodge, J. S. (2021). Maximum-likelihood parameter estimation in terahertz time-domain spectroscopy. *Optics Express*, 29(4), 4912–4926. <https://doi.org/10.1364/OE.417724>
- Neu, J., & Schmittenmaer, C. A. (2018). Tutorial: An introduction to terahertz time domain spectroscopy (THz-TDS). *Journal of Applied Physics*, 124(23), 231101. <https://doi.org/10.1063/1.5047659>
- Peretti, R., Mitryukovskiy, S., Froberger, K., Mebarki, M. A., Eliet, S., Vanwolleghem, M., & Lampin, J.-F. (2019). THz-TDS Time-Trace Analysis for the Extraction of Material and Metamaterial Parameters. *IEEE Transactions on Terahertz Science and Technology*, 9(2), 136–149. <https://doi.org/10.1109/TTHZ.2018.2889227>
- Tayvah, U., Spies, J. A., Neu, J., & Schmittenmaer, C. A. (2021). Nelly: A User-Friendly and Open-Source Implementation of Tree-Based Complex Refractive Index Analysis for Terahertz Spectroscopy. *Analytical Chemistry*, 93(32), 11243–11250. <https://doi.org/10.1021/acs.analchem.1c02132>