

Engineering Aspects of Terahertz Time-Domain Spectroscopy

by

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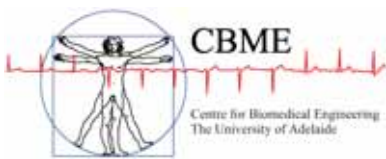
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Abstract

Terahertz time-domain spectroscopy (THz-TDS) is a technique capable of measuring optical constants of materials with T-ray frequencies, bounded between 0.1 and 10 THz. Owing to the infancy of the technology, much work has to be carried out to improve its utility and reliability. Engineering aspects become vital to support its operation that relies on physical phenomena. This thesis, in the arena of engineering, encompasses a variety of original THz-TDS projects, which aim for (**Part I**) signal enhancement and classification, (**Part II**) system evaluation and optimisation, and (**Part III**) T-ray optics:

Part I is relevant to enhancement and classification of T-ray signals via digital signal processing. In one project, information underlying T-ray signals is enhanced through numerical removal of unwanted artefacts that are introduced by the response of water vapour during the measurement. In another project, machine learning is recruited in classification of visually indistinguishable T-ray signals probing materials of the same general class.

Part II focuses on THz-TDS systems with a particular interest in the measurement precision. An ISO standard for the evaluation of measurement uncertainty is adopted for assessing the uncertainty in THz-TDS measurements. The result is an analytical uncertainty model, which allows an improvement in the measurement precision through optimisation of a model parameter in the subsequent work.

Part III involves design, fabrication, and characterisation of THz-TDS hardware components, i.e., antireflection windows and multilayer interference filters. The designs are based upon conventional optical interference theory. Despite that, required materials and fabrication processes are completely different from those used in optics due to the distinctive operating wavelengths, which dictate material responses and structural dimensions.

In addition to these parts of the original contributions, the thesis offers an introductory background to THz-TDS, in the areas of hardware, applications, and data processing.

Statement of Originality

This work contains no material that has been accepted for the award of any other degree or diploma in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published or written by another person, except where due reference has been made in the text.

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December 20, 2009

Signed

Date

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W. Withayachumnankul

Conventions

Typesetting This thesis is typeset using the L^AT_EX2e software. T_EXnicCenter is used as an effective interface to L^AT_EX.

Referencing The Harvard style is used for referencing and citation in this thesis.

Spelling Australian English spelling is adopted, as defined by the Macquarie English Dictionary (Delbridge 2001).

System of units The units comply with the international system of units recommended in an Australian Standard: AS ISO 1000—1998 (Standards Australia Committee ME/71, Quantities, Units and Conversions 1998).

Physical constants The physical constants comply with a recommendation by the Committee on Data for Science and Technology: CODATA (Mohr and Taylor 2005).

Frequency band definition It is preferential to refer to the spectrum band from 0.1 to 10 THz as 'T-rays', according to an argument by Abbott and Zhang (2007), rather than 'terahertz'. However, 'terahertz time-domain spectroscopy—THz-TDS' and 'terahertz gap' are acceptable owing to the general acceptance.

Publications

Journal publications

- WITHAYACHUMNANKUL-W., FISCHER-B. M., FERGUSON-B., DAVIS-B. R., AND ABBOTT-D. (2009). A systemized view of superluminal wave propagation, *Proceedings of the IEEE*, (Accepted, 23-09-2009).*
- WITHAYACHUMNANKUL-W. AND ABBOTT-D. (2009). Metamaterials in the Terahertz Regime, *IEEE Photonics Journal*, **1**(2), pp. 99–118. **(Invited)**.*
- WITHAYACHUMNANKUL-W., FISCHER-B. M., AND ABBOTT-D. (2008). Numerical removal of water-vapour effects from THz-TDS measurements, *Proceedings of the Royal Society A: Mathematical, Physical & Engineering Sciences*, **464**(2097), pp. 2435–2456.
- WITHAYACHUMNANKUL-W., FISCHER-B. M., LIN-H., AND ABBOTT-D. (2008). Uncertainty in terahertz time-domain spectroscopy measurement, *Journal of Optical Society of America B: Optical Physics*, **25**(6), pp. 1059–1072.
- WITHAYACHUMNANKUL-W., FISCHER-B. M., AND ABBOTT-D. (2008). Material thickness optimization for transmission-mode terahertz time-domain spectroscopy, *Optics Express*, **16**(10), pp. 7382–7396.
- WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2008). Quarter-wavelength multilayer interference filter for terahertz waves, *Optics Communications*, **281**(9), pp. 2374–2379.
- WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2007). Retrofittable antireflection coatings for T-rays, *Microwave and Optical Technology Letters*, **49**(9), pp. 2267–2270.
- WITHAYACHUMNANKUL-W., PNG-G., YIN-X. X., ATAKARAMIANS-S., JONES-I., LIN-H., UNG-B. S. Y., BALAKRISHNAN-J., NG-B. W.-H., FERGUSON-B., MICKAN-S. P., FISCHER-B. M., AND ABBOTT-D. (2007). T-ray sensing and imaging, *Proceedings of IEEE*, **95**(8), pp. 1528-1558. **(Invited)**.
- WITHAYACHUMNANKUL-W., FERGUSON-B., RAINSFORD-T., MICKAN-S. P., AND ABBOTT-D. (2006). Direct Fabry-Pérot effect removal, *Fluctuation and Noise Letters*, **6**(2), pp. L227–L239.*
- WITHAYACHUMNANKUL-W., FERGUSON-B., RAINSFORD-T., MICKAN-S. P., AND ABBOTT-D. (2005). Simple material parameter estimation via terahertz time-domain spectroscopy, *IEE Electronics Letters*, **41**(14), pp. 800–801.*

Conference publications

- WITHAYACHUMNANKUL-W., UNG-B. S. Y., FISCHER-B. M., AND ABBOTT-D. (2009). Measurement of linearity in THz-TDS, *Proceedings IRMMW-THz*, Korea, DOI: 10.1109/ICIMW.2009.5324721.*
- WITHAYACHUMNANKUL-W. AND ABBOTT-D. (2008). Survey of terahertz metamaterial devices, *Proceedings SPIE Smart Structures, Devices, and Systems IV*, Melbourne, Australia, **7268**, article number 72681Z.*
- WITHAYACHUMNANKUL-W., FISCHER-B. M., AND ABBOTT-D. (2008). Optimization of material thickness for THz-TDS, *Proceedings IRMMW-THz*, USA, DOI: 10.1109/ICIMW.2008.4665677.
- LIN-H., WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2008). Gas recognition with terahertz time-domain spectroscopy and reference-free spectrum: a preliminary study, *Proceedings IRMMW-THz*, California, USA, DOI: 10.1109/ICIMW.2008.4665829.*
- WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2007). Transmission characteristic of T-ray multilayer interference filter, *Proceedings SPIE Photonics: Design, Technology, and Packaging III*, Canberra, Australia, **6801**, article number 68011G.
- NG-D., WONG-F. T., WITHAYACHUMNANKUL-W., FINDLAY-D., FERGUSON-B., AND ABBOTT-D. (2007). Classification of osteosarcoma T-ray responses using adaptive and rational wavelets for feature extraction, *Proceedings SPIE Complex Systems II*, Canberra, Australia, **6802**, article number 680211.*
- LIN-H., WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2007). Gas recognition with terahertz time-domain spectroscopy and spectral catalog: A preliminary study, *Proceedings SPIE Terahertz Photonics*, Beijing, China, **6840**, article number 68400X.*
- WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2007). T-ray multilayer interference filter, *Proceedings IRMMW-THz*, Cardiff, UK, pp. 307–308.
- LIN-H., WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2007). THz time-domain spectroscopy uncertainties, *Proceedings IRMMW-THz*, Cardiff, UK, pp. 222–223.
- WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2007). Removal of water-vapor-induced fluctuations in T-ray signals: A preliminary study, *Proceedings SPIE Noise and Fluctuations in Photonics, Quantum Optics, and Communications*, Florence, Italy, **6603**, article number 660323.
- WITHAYACHUMNANKUL-W., LIN-H., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2007). Analysis of measurement uncertainty in THz-TDS, *Proceedings SPIE Photonic Materials, Devices, and Applications II*, Gran Canaria, Spain, **6593**, article number 659326. **(Invited)**.
- WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2006). Retrofittable T-ray antireflection coatings, *Proceedings SPIE Micro- and Nanotechnology: Materials, Processes, Packaging, and Systems III*, Adelaide, Australia, **6415**, article number 64150N.
- WITHAYACHUMNANKUL-W., FISCHER-B. M., MICKAN-S. P., AND ABBOTT-D. (2006). Thickness determination for homogeneous dielectric materials through THz-TDS, *Proceedings IRMMW-THz*, Shanghai, China, p. 448.*

WITHAYACHUMNANKUL-W., FERGUSON-B., RAINSFORD-T., FINDLAY-D., MICKAN-S. P., AND ABBOTT-D. (2005). Classification of osteosarcoma via terahertz time-domain spectroscopy, *Proceedings IFMBE International Conference on BioMedical Engineering (ICBME)*, **12**, Singapore. (CD only).

WITHAYACHUMNANKUL-W., FERGUSON-B., RAINSFORD-T., FINDLAY-D., MICKAN-S. P., AND ABBOTT-D. (2005). T-ray relevant frequencies for osteosarcoma classification, *Proceedings SPIE Photonics: Design, Technology, and Packaging II*, Brisbane, Australia, **6038**, article number 60381H.

RAINSFORD-T., PNG-G. M., **WITHAYACHUMNANKUL-W.**, FERGUSON-B., MICKAN-S. P., AND ABBOTT-D. (2005). T-rays in biomedicine and security, *Proceedings IEEE Lasers & Electro-Optics Society (LEOS) Annual Meeting*, Sydney, Australia, pp. 116–117. (Invited).*

WITHAYACHUMNANKUL-W., FERGUSON-B., RAINSFORD-T., MICKAN-S. P., AND ABBOTT-D. (2005). Material parameter extraction for terahertz time-domain spectroscopy using fixed-point iteration, *Proceedings SPIE Photonic Materials, Devices, and Applications*, Sevilla, Spain, **5840**, pp. 221–231.*

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