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A novel robotic THz spectroscopy system and full wave analysis of THz wave-matter interaction*

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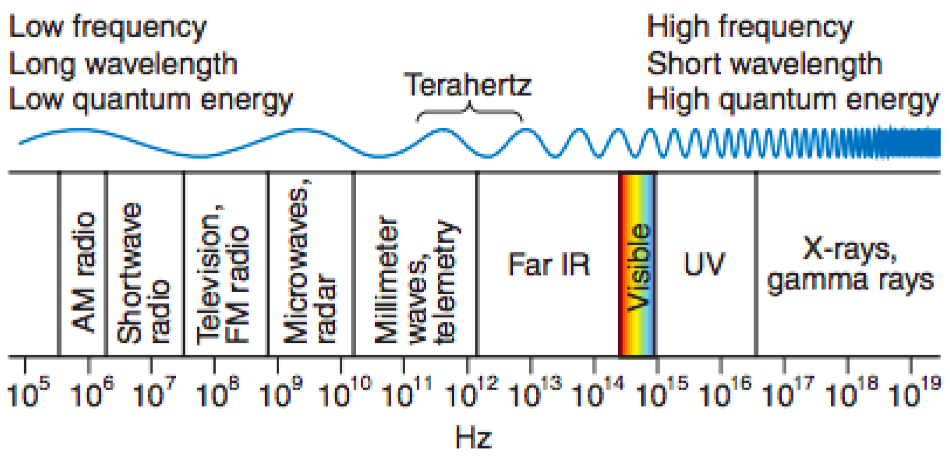
Introduction

- **Terhertz region (100 GHz-10THz):** Inaccessible for many years
  - Efficient sources and sensitive detectors are now available
- **Terahertz (THz) sensing** is becoming popular now a days and **THz time domain spectroscopy (TDS)** is a widely used sensing technique with many applications [JIMTW 36, 235 (2015)].
- Its penetration depth is better than IR and spatial resolution is better than microwaves.



- THz-TDS is getting rapid attention in recent years

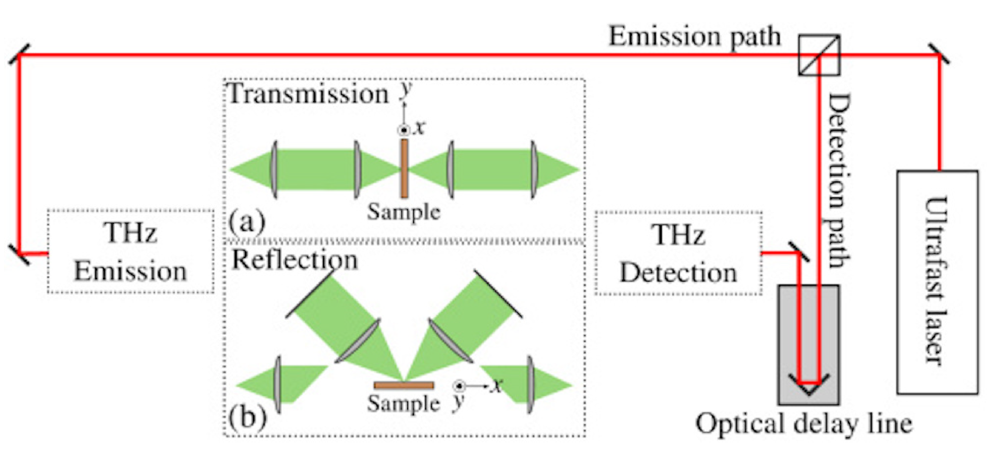
Motivation

- **THz-TDS in reflection geometry** is desired to study the irregular surfaces. However, there are two main challenges:
  - Sample surface doesn't stay in focal plane of the device
  - Angle of beam incidence deviate from normal incidence.
- A robotic manipulator is a solution to the meet the challenges.
- Great advantage of THZ-TDS technique is to obtain timing information of the returning pulse which anables us to determine complex refractive index and dielectric constant of the material.
- This work is focused on realizing a novel robotic THz-TDS system which could be used for imaging of arbitrary shaped samples. The focus would be on cultural heritage and archaeological artefacts.
- The mechanism of **THz wave-matter interaction** would also be studied by theoretical full wave analysis for better interpretation of THz wave propagation characteristics in materials.

Application Areas of THz Technology

- Spectroscopy and imaging
- Non-destructive testing
- Quality inspection in industry
- Detection of hazardous fluids
- THz combs and ultrafast switching
- Coatings and layers inspection
- Atmospheric research
- Concealed metal detection
- And many more

Schematic of a THz-TDS System



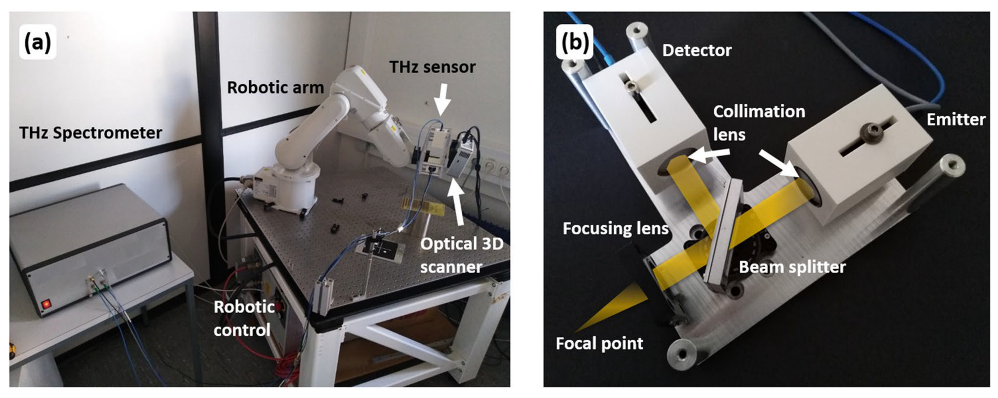
- Includes a fibre-coupled Tx and Rx, nm laser, THz optics, delay line, and acquisition platform, THz optics, etc. [Fig.: AOP (2018)]
- Set up is possible in ransmission and reflection geometry
- Industry-proven sensors and spectrometers are available
- A customized system cab be devised with flexibility

Robot-assisted THz-TDS systems

- Conventionally, THz-TDS systems uses raster scanning scheme for imaging purposes
- This is successful in 2D translation of flat surfaces in the focal plane
- For thick or highly absorbing materials, only reflection geometry with a robotic aid can be successful with variable methods of data acquisition
- **THz emitter and receiver** can be mounted on a robotic system
- Fibre-coupled data aquisition and scanning systems are conveniently mounted
- Commercial THz spectrometers are used for analysis
- Full control over field of view of THz sensor and angle of incident beam is possible in new designs

Robotic THz Systems for Cultural Heritage

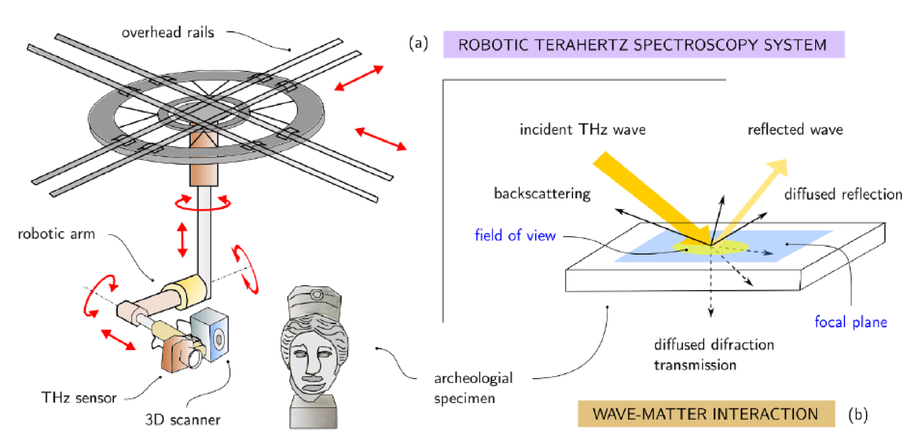
- **Recent setup: Stubling et al.** [JIMTW (2017)]



  - **Limitations:** Field of view, focal plane of the beam, incidence angle
- **Need:** Better control over focal plane with large scanning angle
- **Additional:** Prior knowledge of some wave dependencies and material properties may be helpful
- **This work:** Proposes a robotic THz manipulator with improved or new features for spectroscopy and imaging applications

Concept of novel robotic-THz spectroscopy and imaging system

- **Schematic diagram:** New proposed design



- Distance between Tx and Rx (sensor) & angles are controllable
- Scanner is used separately for beam path reconstruction and surface profile
- The acquisition platform (spectrometer incl. fs laser, delay line, bias voltage, A/D converter, PC and software) is not shown
- The TDS allows not only the intensity, but also the direct measurement of the electric field as a function of the delay
- The sensor head is kept perpendicular to the measurement point in usual designs
- The pulse amplitude reduces by reflection, absorption, and scattering, and the pulse is delayed due to the index of refraction
- The spectral information is fed to spectrometer and acquisition system for imaging data

THz Wave-Matter Interaction

- **Amplitude and phase information in TDS**
  - THz waves interacting with an object respond to material characteristics by changing their intensity & temporal behavior
  - From absorption and dispersion of a probing THz pulse one can derive information on the material thickness & density
  - By measuring the amplitude and the phase of the pulse at well-defined positions, a THz image of an object can be reconstructed
  - With an additional spectral analysis even different material components can be identified

Theoretical Study

- **Modeling and analysis**
  - THz wave propagation in matter
  - Development of full wave computational approach(es)
  - Full wave analysis
  - Measuring material properties
- **Wave interaction phenomena involved**
  - Reflection and scattering
  - Wave-optics phenomena (tunneling, diffraction, refraction, standing wave formation, inhomogeneities, etc)
  - wave-particle interaction/kinetic effect

Full Wave Analysis

- **Solves Maxwell's equation as a boundary-value problem**
- **In a non-dispersive medium:** $\overleftrightarrow{\epsilon}(\boldsymbol{r})$
  - Stationary full wave analysis: $\boldsymbol{E}(\boldsymbol{r})\,e^{-i\omega t}$

$$\nabla\times\nabla\times\boldsymbol{E}-\frac{\omega^2}{c^2}\overleftrightarrow{\epsilon}\cdot\boldsymbol{E}=0$$

  - Quasi-optical analysis: $\boldsymbol{E}(\boldsymbol{r},t)\,e^{-i\omega t}$

$$i\frac{2\omega}{c^2}\overleftrightarrow{\epsilon}\cdot\frac{\partial\boldsymbol{E}}{\partial t}=\nabla\times\nabla\times\boldsymbol{E}-\frac{\omega^2}{c^2}\overleftrightarrow{\epsilon}\cdot\boldsymbol{E}$$

  - Finite-difference time-domain (FDTD) analysis: $\boldsymbol{E}(\boldsymbol{r},t)$

$$-\frac{1}{c^2}\overleftrightarrow{\epsilon}\cdot\frac{\partial^2\boldsymbol{E}}{\partial t^2}=\nabla\times\nabla\times\boldsymbol{E}$$

- **In a dispersive medium:** $\overleftrightarrow{\epsilon}(\omega,\boldsymbol{k};\boldsymbol{r})$ is more complicated
- **For 10 THz wave:** λ=0.03 mm; required mesh size=0.005 mm
- Very large computational resource is needed for 10 THz wave for 3D, even for 2D analysis
- **For 1 THz wave:** $\lambda = 0.3$ mm; Maximum mesh size = 0.05 mm **2D analysis** with image size = 50 cm requires variable memory size = 0.5 GB, and matrix coefficient = 2.5 GB $\Longrightarrow$ reasonable computational requirements and memory
- Numerical code results for the above 3 approaches would be compared quantitatively to obtain the best scheme for analysis
- We would start with 2D analysis and a small size of 3D analysis for pulsed THz wave. All three full wave approaches could be started in the 1 THz range and extension to higher frequency range by parallel processing could be developed

Summary

- We have proposed a novel robotic THz time domain spectroscopy and imaging system. to maximally improve the constraints of beam incidence angle, field of view and focal plane of the earlier devices
- A prototype device would be realized and tested for spectroscopic and imaging study, initially for simplest material and extending to selected materials in archaeology.
- The propagation characteristics of THz wave would be studied theoretically by full wave analysis. This should result in better interpretation of THz wave propagation and wave-matter interactions and to investigate certain material properties.