Terahertz Time Domain Spectroscopy for molecules inspection: water vapor and drugs

Enrique García-García[1], Yahya Moubarak Meziani[2], Jesús Enrique Velázquez-Pérez[2] and Jaime Calvo-Gallego[3]

[1]Centro de Lásers Pulsados (CLPU), Edificio M3, Parque Científico USAL; Calle Adaja s/n, 37185 Villamayor, Salamanca, Spain
[2]Departamento de Fisica Aplicada, Plaza de la Merced s/n, Universidad de Salamanca, 37008 Salamanca, Spain
[3]Escuela Politécnica Superior de Zamora, Avda. Cardenal Cisneros, 34, Universidad de Salamanca, 49022 Zamora, Spain

egarcia@clpu.es

Abstract
In this paper we report on an experimental study of the spectral response of different compounds in the THz range. We set up a THz Time Domain Spectroscopy System (TDS) that uses a Ti:Sapphire femtosecond laser and a pair of LTD GaAs photoconductive antennas for THz generation and detection. The THz TDS set up was validated through the matching of the main lines of the water vapor spectra in the 0.1-3THz range against the HITRAN database. Finally, the THz spectra of two commercial chemical compounds (paracetamol and ibuprofen) were obtained; the large difference found between the two spectra will easily allow to distinguish between both substances. Further work will be necessary to understand the fingerprints of those substances.

Introduction
Terahertz radiation is located in the spectral region 0.1-10 THz (3 mm - 30 µm, 3 cm^{-1} - 300 cm^{-1}) between the microwave and the infrared part of the electromagnetic spectrum. The interest in this spectral region comes from the fact that many substances have a “fingerprint” within this region. Several studies performed on different materials, from medical drugs to explosives, have showed this unique behavior [1-4]. Experiments carried out by Grichkowsky et al [5] showed the potential for THz spectroscopy of photoconductive switches by resolving in time the THz pulse transmitted through a sample, following the Time Domain Spectroscopy (TDS) scheme.

System Description.
We set up of a THz-TDS system where the emission and detection are performed by photoconductive antennas [6] (low temperature grown GaAs) triggered by ultra-short laser pulses. A substrate lens fabricated from high resistance Silicon is attached to the backside of each antenna to guide the THz radiation toward the detector. Figure1 shows the optical layout of the system. The pumping laser pulse is a Ti:Sapphire oscillator at 780-810 nm, 60-80 fs and 50-150 mW output power at 80 MHz pulse repetition rate. The system covers a range from 100 GHz until 3 THz (limited by the absorption of a pair of low density polyethylene focalization lenses) and the emitted power of the THz radiation is around 10 µW.

The antenna is polarized in DC to obtain an internal electric field of 4kV/cm. When the fs pulse the first antenna, a bunch of free carriers is generated and then accelerated under the stationary electric field. The relaxation of the free carriers generates the terahertz pulse. Detection follows the same principle but, instead of applying an external DC bias, the incoming THz radiation creates a field in the second antenna that provides a DC voltage. Both processes, emission and detection, are generated in a pump and probe scheme, thus both processes are coherent. The detection is achieved by sweeping the delay of one of the laser pulse arms. The signal measured in the detector is proportional to the THz electric field itself, instead of to its amplitude. Therefore, via Fourier analysis we can extract both the spectral amplitude and phase of the pulse. This allows the extraction of the complex electrical permittivity without carrying a Kramers-Kronig analysis [7]. A typical temporal and spectral profile is shown in Fig.2. Fourier transform allows us to extract the THz transmitted electrical field on a sample when we evaluate the ratio between the sample and reference measurements.

Experimental results
Measurement of water vapor has been performed by determining the transmitted electrical field on air with a relative humidity close to 40%. The result can be seen in Fig. 3. The decay of the spectra when the frequency increases exhibits several peaks that have been correlated with the absorption lines of water (only for lines with an intensity ≥10^{20} cm/(molecule cm^2)) obtained from HITRAN's database.

We also present the transmission spectra for two different commercial drugs, in particular paracetamol and ibuprofen, in Fig.4. The excipient may also have an influence on the obtained spectra and generate some of the observed peaks. On the other hand, there is a large difference between the spectra of both samples that indicates the ability of the technique to distinguish between drugs in the studied THz range. Further work will be carried out to understand the position and intensity of different peaks. We believe that this method could bring new information on nanoscale materials, like nanoparticles, nanowires, etc.

Summary and Conclusions

We have performed several studies of TDS on different samples. We have been able to correctly obtain the absorption lines of water from vapor from 0.1 THz up to 3 THz in agreement with well-established data bases. Additionally, we have experimentally shown that the technique allows the discrimination between different chemical substances. Future work will try to develop a THz-TDS system using nanometric Field Effect Transistors as source/detector of THz radiation.

Acknowledgemets

This work was partly funded by Ministerio de Ciencia e Innovacion (MICINN) under Grant TEC2008-02281 and Junta de Castilla y León under Grant SA061A09.

References

[1] R. Woodward, B. Cole, V. Wallace, R. Pye, D. Arnone, E. Linfield, and M. Pepper, Physics in Medicine and Biology, **47** no. 21, (2002), 385.
[2] K. Kawase, Y. Ogawa, Y. Watanabe, and H. Inoue, Opt. Express, **11** no. 20, (2003), 2549.
[3] Shen, T. Lo, P. Taday, B. Cole, W. Tribe, and M. Kemp, Appl. Phys. Lett., **86**, (2005), 241116
[4] B. Ferguson and X. Zhang, Nat. Mater., **1** no. 1, (2002), 26
[5] M. van Exter and D. Grichkowsky, Phys. Rev. B 41, (1990), 12140.
[6] P.R. Smith, D.H. Auston, and M.C. Nuss, IEEE J. of Quantum Electronics, **24**, (1988), 255.
[7] S. Nashima, O. Morikawa, K. Takata, and M. Hangyo, J. Appl. Phys., **90**, No. 2, (2001), 837

Figures

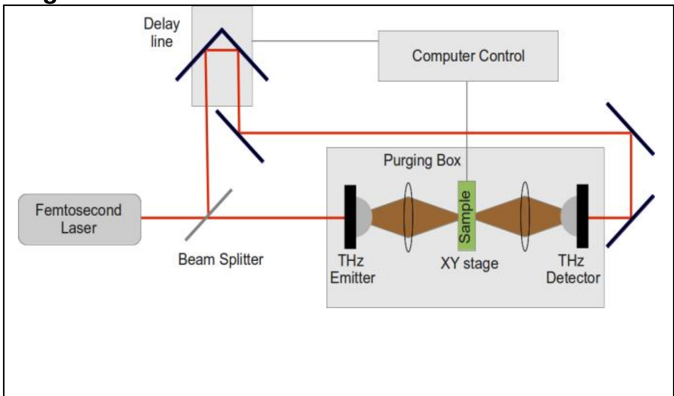

Figure 1: Scheme of the THz-TDS system.

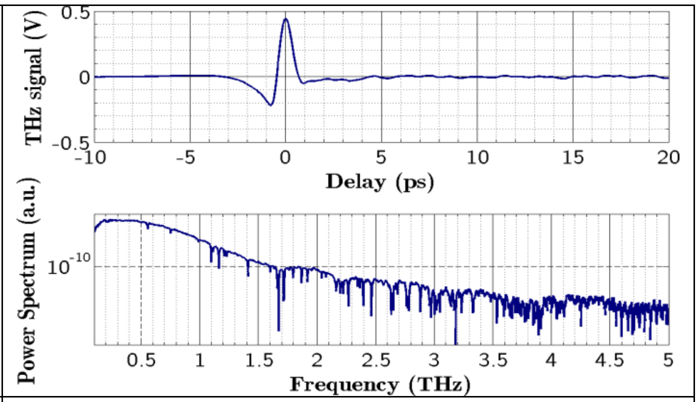

Figure 2: Temporal (up) and spectral (bottom) profile of the THz electrical field transmitted on air.

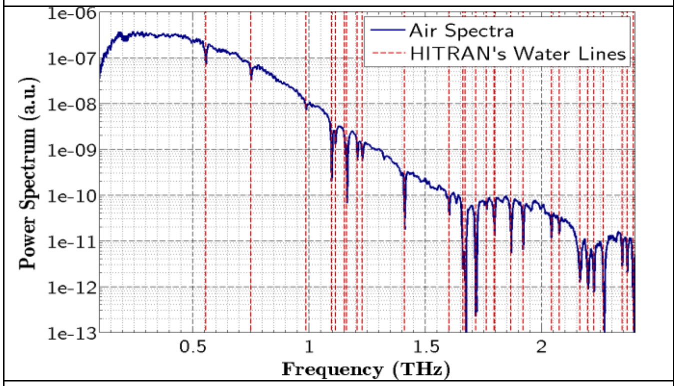

Figure 3: Water vapor power spectrum. The vertical lines are the absorption lines of water with an intensity bigger or equal than 10^20 cm/(molecule cm^2) from HITRAN's database

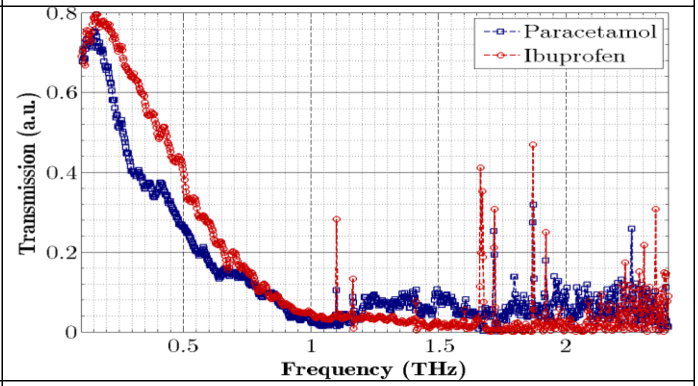

Figure 4: Transmission spectra of two different drugs.