Terahertz Electronics for Chemical and Biological Warfare Agent Detection

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Abstract- The capability of solid-state electronics within the terahertz frequency regime is reviewed and assessed. Recent developments in chemical and biological science are presented that provide important insight and motivations for future uses of THz electronics in spectroscopic sensing. Finally, the impact of new advances in nanotechnology and molecular physics on the detection of chemical and biological warfare agents is addressed.

Introduction

In this final year of the twentieth century, the solid-state electronics capability within the terahertz (THz) frequency regime remains extremely limited from a basic signal source and systems perspective. The relative limited development of semiconductor-based electronic circuits in the THz band, defined here as the portion of the submillimeter-wavelength electromagnetic (EM) spectrum between approximately 1 mm (300 GHz) and 100 μ m (3 THz), may be attributed to the confluence of two fundamental factors. First, very challenging development and engineering problems are present in this quasi-optical regime where EM wavelength is on the order of component size. Second, the practical and scientific applications of this shorter-wavelength microwave region have been restricted to a few specialized fields. However, recent advances in nanotechnology, molecular chemistry and biological science have already begun to chart the course for new and important applications of THz electronics in the coming twenty-first century.

A brief review of the current state-of-the-art in THz electronics and THz frequency regime applications is first given for historical perspective. This paper then focuses on recent developments in chemical and biological science that provides important insight and motivations for future uses of THz electronics in spectroscopic sensing. Here, the utilization of the THz frequency regime for the detection of chemical and biological warfare agents is emphasized. Finally, the impact of new advances in nanotechnology and molecular physics on sensing is addressed.

Background

While the THz regime offers a number of general advantages (e.g., wider bandwidth, improved spatial resolution, and compactness) for remote sensing technology, applications in molecular spectroscopy has been the major driving force for the development of the submillimeter-wave region between microwaves and the infrared. All spectroscopy relies upon the interaction of EM fields with matter and the major value of the THz regime is manifest by the abundant density of rotational energy levels of free molecules that occur naturally in this spectral region. Hence, the rich potential of THz spectroscopy for the study of small molecules (with a limited number of clearly discernable rotational lines) is well known: to astrophysical and astrochemical scientists [1]. Furthermore, very recent investigations [2] have shown that the THz regime can be extremely useful

for the study, analysis, and detection of relatively large (> 100 AMU) molecules within a laboratory environment (i.e., at low temperature and pressures). While these facts have provided strong motivation for the development of THz technology suitable for the laboratory (e.g., T-Rays [3], BWO's [2], etc.), advances in semiconductor-based technology that is integratable, miniaturizable and cost-effective, has been somewhat limited. The advantages of passive millimeter-wave imaging, primarily for its potential in military surveillance, have been an adequate motivation for the development of monolithic microwave integrated circuits (MMIC's) up to 300 GHz, below which the atmosphere remains relatively transparent [4]. In addition, prospects in radio astronomy, space-based earth observation systems, satellite communications, very-short-range land-based communications/guidance etc., [5,6] albeit somewhat limited, have provided some impetus for the development of compact solid-state sources at THz frequencies. Specifically, while the earliest focus in THz source technology has been on vacuum devices [7] there is, for example, substantial ongoing research into Schottky diode multipliers [8], LTG GaAs photomixers [9], GaAs Tunnel diodes [10] and HEMT-based plasma-wave generation [11]. However, a real question that remains is whether there exists commercial and/or Department of Defense (DoD) applications of THz technology that strongly justify the further development of very high frequency solid-state

electronics [12]. The recent investigations into T-Ray [3] and Electro-Optical [13] based imaging have demonstrated the potential of THz spectroscopy for probing the electronic, vibronic, and compositional properties of polar materials in the solid, liquid and gas phase. The applications demonstrated also include the spectral analysis of organic materials (e.g., distinguishing cancer in human tissue), concealment devices (e.g., to find voids in plastic containers), flames and flows. Hence, quite a few commercial and military related uses of THz technology have been revealed by these laboratory studies. However, cost and portability are issues for these laser-based spectroscopic systems and one might still question whether there are compelling reasons for the development of a THz electronics capability.

Warfare Agent Detection at THz Frequency

The recent proliferation of chemical and biological (CB) agents as instruments of warfare and terrorism has lead the DoD to rank the development of early-warning systems for biological, and then chemical, as the *highest priorities* [14]. Very recent spectroscopic studies at millimeter-wave and submillimeter-wave have indicated that DNA (and possibly other cellular material) possesses large numbers of unique resonances due to localized phonon modes [15]. The data given in Figs. 1-3 illustrates the strong potential of THz spectroscopy

Figure 1. Spectra of herring (H) and salmon (S) DNA in the very-far IR (d is thickness).

Figure 2. Spectra of herring (H) and salmon (S) DNA enhanced by film preparation procedure.

Figure 3. Anthrax simulate (BG) exhibited unique features above ~1 THz, in contrast to DNA.

Figure 5. FTIR-generated spectrum for the warfare agent, Soman.

Figure 4. FTIR-generated spectrum for the warfare agent, Sarin.

as a new approach for point detection of biological agents (i.e., in the ~300-750 GHz). Here, the spectra reveals unique contributions from the localized phonons, arising from DNA base-pair interactions, that is absent from the far infrared data (i.e., > ~1 THz). Studies at W-band (75-110 GHz) have revealed similar results. Hence, a millimeter-wave approach may offer a technique to achieve standoff-detection capability in concert with the more discriminating THz identification technology. The serious military threat of large toxic molecules (e.g., Sarin) has also motivated microwave spectroscopic

Figure 6. Calculated higher-frequency rotational spectrum for Sarin

studies that have, for the first time, made rotational-state assignment of chemical warfare agents. The assignment of the ground-state rotational energies, as given for Sarin and Soman in Figs. 4-5, is very important for two reasons. First, this work establishes a microwave-based approach for the detection and identification of chemical agents that is highly species-specific and applicable at extremely low concentration [16]. However, while this microwave-based approach is somewhat

portable, it does require a tunable Fabry-Perot cavity (for sensitivity) and low-pressure conditions to resolve the rotational lines. Second, these studies allow for the *accurate* calculation of the higher-frequency rotational spectrum as given in Fig. 6. Here, the very familiar phenomenon of increasing interaction strength with frequency is observed. There are two phenomena that cause the intensity profile to reach a maximum value in the region of 300 GHz. One is the increase in rotational line strength with frequency that varies as the square of the frequency and the second is the thermal Boltzmann distribution. In addition, at a finer detail, the a-type rotational transitions tend to clump at particular values due to state degeneracies. This leads to further increases of peak absorption in certain frequency regions. Hence, THz spectroscopy offers advantages for chemical detection and may be made viable if pressure broadening is controlled and methods are developed to provide rapid survey scans of broad spectral regions.

Conclusions

At this particular stage, new research utilizing THz spectroscopy has laid a preliminary foundation for new warfare agent detection *and analysis* methods. However, there remains much work ahead to fully identify a robust THz-based methodology. Specifically, any CB agent detection scheme requires the interrogation of a *microscopic* molecule and therefore will present very stringent specificity and sensitivity problems. Fortunately, the scientific community has been addressing this general problem for some time. For example, novel methods are being developed to assemble nanoparticles into macroscopic materials that may provide a means for linking microscopic molecules to sensing devices [17,18]. Therefore, the *successful* detection of CB warfare agents will most certainly require a fusion of a robust THz electronics capability for species specificity and a molecular nanoelectronics expertise for microscopic sensitivity [19].

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