High-Precision Probing of Molecules Using THz CMOS Chips: Principles and Applications in High-Accessibility Sensors and Clocks

(Invited Talk)

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Abstract

Polar molecules posses quantized rotational energy states. A transition between two states can be excited when an externally-applied electromagnetic (EM) wave matches the rotational resonance frequency. Interestingly, the rotational energy is normally very low, which makes the transitions locate mostly in the millimeter-wave and low-THz bands. At certain low pressure levels, when the linewidth of the transitions is mainly limited by the Brownian motion of the molecules, the quality factor of the lines is close to one million! That enables gas sensing with a selectivity that is much higher than in mass spectroscopy and infrared (IR) spectroscopy. The high spectral concentration of the transition energy also increases the SNR of the detection. Unfortunately, due to the long-existing challenges in the implementation of THz hardware, THz rotational spectroscopy was previously only adopted in astronomical instruments (for inter-stellar dust detection) and bench-top gas analyzers (for gas mixture identifications).

Recent progress of CMOS-based THz electronics makes it possible to realize molecular sensing using low-cost silicon chips. In 2017, we demonstrated a CMOS-based spectrometer using a dual-frequency-comb architecture with a seamless coverage from 220 to 320 GHz [1]. It breaks the conventional performance tradeoff between bandwidth and efficiency, and realizes record total radiated power (5.3 mW) and sensitivity (noise figure NF=15$\sim$20 dB) in CMOS THz circuits. False-alarm-free detection of gas mixture with a sensitivity (without any pre-centration of sample) of a few *ppm* (part-per-million) is demonstrated [2], showing the feasibility of high-performance while ultra-portable gas sensors for breath analysis, pollution monitoring, etc.

Next, we further apply the CMOS spectrometer technology into the area of high-precision time keeping, which was previously dominated by costly atomic clocks invovling high-complexity electro-optical constructions. By probing the exact low-THz transition frequency of carbonyl sulfide (OCS), we innovate a chip-scale molecular clock using a fully-electronic CMOS spectrometer [3], [4]. The OCS gas is encapsulated inside a single-mode waveguide, enabling miniaturization of the clock. Consuming only 66 mW of power, the clock chip delivers an Allan deviation of 3×10^{-10}, and is expected to further increase the stability to the 10^{-12} level using an OCS gas cell with low out-gassing/leakage and improved wave coupling [4]. In this talk, the principles and designs of the molecular clock will be introduced. In addition, recent studies and experimental results of the clock regarding its robustness against temperature change and external magnetic field are presented [5]. With the elimination of the need for any temperature-stabilizing oven or magnetic shield, the molecular clock offers a highly-simplified solution for miniature frequency references, making it possible to realize atomic-clock-grade time keeping in mainstream, cost-sensitive equipment. With the ever-increasing operation speed of CMOS transistors, as well as the recent MEMS-based THz waveguide technologies [6], we believe a monolithic molecular clock in standard CMOS process is on the horizon (Fig. 1).

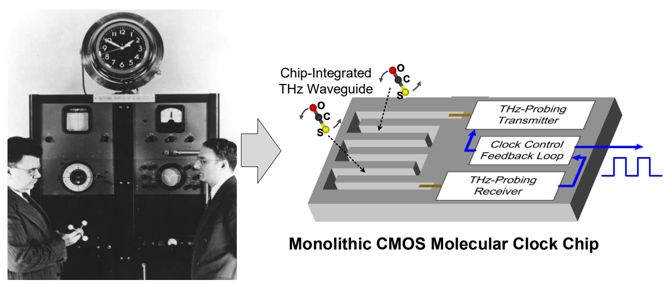

Fig. 1: Evolution from the first ammonia molecule clock in 1949 [7] to a monolithic CMOS carbonyl sulfide molecule clock.

References

[1] C. Wang and R. Han, "Rapid and Energy-Efficient Molecular Sensing Using Dual mm-Wave Combs in 65nm CMOS: A 220-to-320GHz Spectrometer with 5.2mW Radiated Power and 14.6-to-19.5dB Noise Figure," in *International Solid-State Circuit Conference (ISSCC)*, San Francisco, CA, 2017, pp. 18–20.

[2] ——, "Molecular Detection for Unconcentrated Gas with ppm Sensitivity Using Dual-THz-Comb Spectrometer in CMOS," *IEEE Trans. Biomedical Circuits and Systems*, vol. 12, no. 3, pp. 709–721, 2018.

[3] C. Wang *et al.*, "An On-Chip Fully-Electronic Molecular Clock Based on sub-THz Rotational Spectroscopy," *Nature Electronics*, vol. 1, no. 7, pp. 421–427, 2018.

[4] ——, "Chip-Scale Molecular Clock," *IEEE Journal of Solid-State Circuits*, vol. 54, no. 4, pp. 1–13, 2019.

[5] M. Kim *et al.*, "Chip-Scale Terahertz Carbonyl Sulfide (OCS) Clock : An Overview and Recent Studies on Long-Term Frequency Stability of OCS Transitions," *IEEE Transactions on Terahertz Science and Technology*, 2019.

[6] B. Beuerle *et al.*, "A Very Low Loss 220-325 GHz Silicon Micromachined Waveguide Technology," *IEEE Transactions on Terahertz Science and Technology*, vol. 8, no. 2, pp. 248–250, 2018.

[7] M. A. Lombardi *et al.*, "NIST Primary Frequency Standards and the Realization of the SI Second," *NCSL International Measure*, vol. 2, no. 4, p. 74, 2007.