Abstract number: I9
Invited

Multivariate Spectral Analysis in Quartz-Enhanced Photoacoustic Spectroscopy

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Quartz-Enhanced Photoacoustic Spectroscopy (QEPAS) exploits the photoacoustic effect occurring in the modulated light absorption of gas sample, by employing a quartz tuning fork (QTF) as a sharply resonant microphone[1]. In detail, a modulated light source is focused between QTF prongs and sound waves are generated via photoacoustic effect, as schematically depicted in Fig.1.

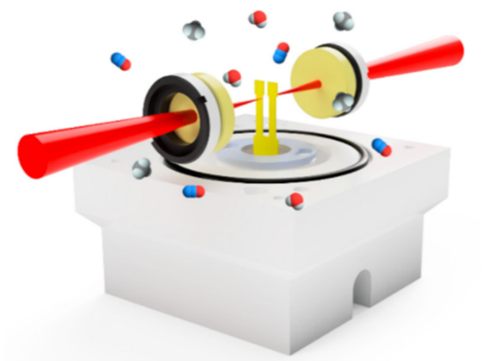

Figure 1: Schematic of a photoacoustic excitation in QEPAS sensing.

The very basic principle of operation for employing a QTF as a sound detector requires the laser modulation frequency to be set at one of the QTF resonance frequencies related to in-plane flexural modes. Thus, when the acoustic wave puts both prongs in their natural oscillation motion, a stress field along the prong is generated. In other words, the laser beam can be treated as a cylindrical acoustic source, inducing prong vibrations due to the pressure wavefronts hitting the prong internal surface. In the elastic regime, the stress field induces a strain field which in turn generates a local polarization of the quartz. Therefore, charges appear on the surface that can be collected by electrical contacts properly deposited along the QTF prong. The strain field as well as piezoelectric charge distribution are mainly localized at the prong clamped end.

Based on an indirect absorption, QEPAS sensing does not need any optical detector and the sound wave detection is wavelength independent. This makes QEPAS technique suitable for multi-gas detection with broadband spectra. QEPAS typically targets isolated absorption features to evaluate the analytes concentrations and avoid interferences from other species contained in the gas matrix. A partially resolved or unresolved spectrum, resulting from the overlap of absorption features of different gases requires a distinct approach. Multivariate Analysis based on Partial Least Squares Regression (PLSR) is combined with QEPAS and here proposed to deconvolve spectral contributions of each component in a multiple-gas mixture characterized by strong overlapping absorption features[2]. PLSR is also dealt with cases when interactions among different components occur, resulting in a spectral correlation that can be efficiently modelled and removed, to retrieve the actual concentration of each component in the mixture.

[1] P. Patimisco, A. Sampaolo, L. Dong, F.K. Tittel, V. Spagnolo, *Appl. Phys. Rev.* **5**, 011106 (2018).
[2] A. Zifarelli, *et al.*, *Anal. Chem.* **92**, 11035 (2020).