Available online at www.sciencedirect.com

SCIENCE DIRECT®

Sensors and Actuators B 116 (2006) 183–191

SENSORS AND ACTUATORS B CHEMICAL

www.elsevier.com/locate/snb

Exploration of the metrological performance of a gas detector based on an array of unspecific infrared filters

R. Rubio[a,*], J. Santander[a], J. Fonollosa[b], L. Fonseca, I. Gràcia[a], C. Cané[a], M. Moreno[b], S. Marco[b]

[a] *Centro Nacional de Microelectrónica (IMB-CSIC), Spain*
[b] *Departament d'Electrònica, Universitat de Barcelona, Spain*

Received 10 July 2005
Available online 25 April 2006

Abstract

The feasibility of a non-dispersive infrared (NDIR) gas detection system based on an array on non-specific detectors is studied in this work. The measurement system, that is intended to be low cost and of reduced dimension, is aimed to the simultaneous quantitative detection of different gases with IR absorption bands in the region of the 1000–4000 cm^{-1}. The detector is a single module that has been already fabricated. It is composed by an array of broadband infrared filters and a matching array of thermopile detectors joint together by means of flip chip. The elements of the filter array are not tuned for the specific measurement of any gas, in opposition to traditional NDIR setups, making necessary the use of multivariate regression techniques (Partial least squares) to predict the gases concentration. A preliminary evaluation of the metrological characteristics of the complete NDIR system is carried out using a realistic model of the system. Two arrays sizes, 3 × 3 and 4 × 4 elements, are studied for the discrimination of a mixture composed by methane, carbon monoxide and carbon dioxide at different concentrations. Prediction errors about tens of ppm are found for an optical path length of 10 cm. In traditional NDIR systems infrared source aging is compensated by means of a reference channel where no absorptions bands are present. Instead, in this in this work these effects are removed using a digital component correction technique.

Keywords: NDIR; Optical gas detection; Thermopile; Thin films filters; Flip chip; Component correction; Drift

1. Introduction

Analytical methods based on infrared spectroscopy are highly selective methods that make the estimation of an analyte in a complex matrix possible. There are four types of instruments for infrared spectroscopy measurements available: dispersive grating spectrophotometers for qualitative measurements, Fourier transform instruments for both qualitative and quantitative measurements, non-dispersive photometers for quantitative determination of organic species in the atmosphere and reflectance photometers for analysis of solids. The size and the price of this kind of instruments are their main drawbacks.

Non-dispersive infrared (NDIR) gas detection systems are based on the detection of the absorption of radiation by analytes at certain wavelengths [1]. Although the relationship between the optical absorption and the gas concentration shows a non-linear behaviour (Lambert-Beer law), optical measurements are, in general, more reliable than solid state gas sensors.

A typical NDIR measurement setup is composed by an infrared source that illuminates the gas to be detected. In most cases these devices use a fixed set of multilayer filters, or filter roulette, limiting the number of simultaneous gases that can be detected. Those filters placed before the infrared detector select the band where the absorption lines of the target substance are placed. The main advantages of this system are high selectivity, the ability to be configured for the measurement of several species by using different selective filters and the immunity to false alarms and poisoning since the detectors are not in direct contact with the gas. In addition, long term stability is improved by the use of a reference band without absorptions. Using this reference band, effects of the infrared source aging can be corrected.

This NDIR measurement method based on the use of selective filters has been already used in commercial devices. Previ-

---

[*] Corresponding author. Tel.: +34 935947700; fax: +34 935801496.
E-mail address: rafael.rubio@cnm.es (R. Rubio).

0925-4005/$ – see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.snb.2006.03.018

ous attempts to build a NDIR micro spectrometer by the use of MEMS structures have been done only recently [2]. Other proposal is based on the use of a Fabry Perot micro spectrometer built using surface micro-machined polysilicon mirrors that are actuated electro statically [3,4]. Tuneable infrared laser differential absorption spectroscopy has been used for years, although recently quantum cascade lasers have been introduced [5]. Also, the dependence of the emission spectra of the IR source on the temperature has been proposed, in this way modulating the temperature of the IR source different emission spectra are achieved and hence acting like a spectrometer [6].

Our goal is to develop a low cost and reduced dimension NDIR analyzer that may be of use for the large number of analytes with absorption bands in the mid infrared. To do so, we propose a *non-selective* optical detection system based on a broadband filter array. Instead of using one selective filter per substance we use an array of filters with different transmittance spectra that cover the interest region (1000–4000 cm^{-1}). As a result of this, a voltage pattern is obtained as the output of the system and multivariate regression techniques should be used to predict the gas concentration.

A model of the system is built to evaluate the ability to discriminate and quantify different mixtures of gases, despite having non-selective sensors. The simulation uses real measured characteristics of all the system elements. To simulate the infrared gas spectrum HITRAN database is used [7]. To illustrate this concept, we prove in this work the feasibility of an array of broadband filters in combination with multivariate regression techniques for the simultaneous detection of three gases (CO, CO_2 and CH_4). Note that although these three gases are used in this work, the scope of applications of these systems is broader and the choice of these gases is due to the fact that their infrared absorbances are well known and available at the HITRAN database, and because of their practical engineering interest.

In the following sections, we will first introduce the measurement system making a short description of all the elements and how they have been modelled. Then, a synthetic experiment will be described, followed by multivariate regression leading to an estimation of the expected accuracy for this system.

A potential drawback of this system is the absence of a reference band to correct source aging or obscuration due to dirtiness. The last section of the paper shows that component correction is an effective way to compensate source drift [8].

2. NDIR system model description

A sketch of the measurement system structure is shown in Fig. 1. The radiation produced by the infrared source passes through a gas chamber and reaches the detector array. Each filter weights in different manner different parts of the spectrum and consequently the thermopile array generates a voltage pattern. This voltage pattern will be subsequently processed to finally estimate the gas concentration by suitable multivariate calibration methods.

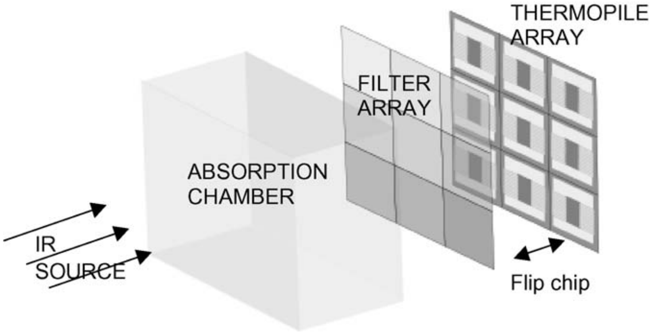

Fig. 1. Gas detection system architecture.

2.1. Infrared radiation source

The radiation source is a commercial device (refelctIR-P1C Ion Optics Waltham, USA). The radiation spectra produced by this device is considered proportional to that of an ideal blackbody heated at the same temperature (850 °C). The spectral irradiance of the source is calculated from Plank's Law [1] using uniform values for the temperature T (850 °C) and the source emissivity ε (0.7). The effective emitting area used is 2 mm^2.

The full angle for 50% of peak power of the IR source, provided by the manufacturer ($\theta_{1/2} = 30^\circ$), allows us to calculate the directivity parameter of the source n assuming a Lambertian distribution: in our case the obtained directivity is 4.8.

$$n = \frac{-\ln 2}{\ln(\cos\theta_{1/2})} \tag{1}$$

2.2. Power transmission

Two zinc selenide lenses, placed in both extremes of the absorption chamber, are used in order to enhance the power transmission. The model considers the dispersion losses between the source and the entrance of the chamber assuming that once inside, the light is only influenced by the gas absorption. The power losses due to the lenses transmission are considered using the transmittances values provided by the manufacturer ($T = 0.9$).

The fraction of the emitted power Φ_E arriving to the entrance of the chamber Φ_D, after a certain optical path length L (distance between the IR emitter and the first lens), is obtained from the partial integration over the solid angle sustained by the lenses respect to the source. We assume that the source is in the focal length of the lens.

This fraction is:

$$\frac{\Phi_\mathrm{D}}{\Phi_\mathrm{E}} = 1 - \cos^{n+1}\left(\arctan\left(\frac{r}{L}\right)\right) \tag{2}$$

where r is the radius of the first lens ($r = 1.27$ cm) of the system and n the directivity parameter of the source. The last lens of the optical system, located between the gas chamber and the detector filters, is devoted to focus the beam to the sensing area of the array. To calculate the fraction of optical power that arrives to each element of the array, we integrate over the portion of solid angle of the beam captured by the corresponding sensitive area.