Algorithm for processing data from a resistive semiconductor gas sensor when it operates in thermal modulation mode

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It is shown that the temperature response of the semiconductor sensor of the resistive principle of action in the gas mixture can be approximated by the sum of concentration responses to individual components of the analyzed gas mixture taking into account their cross sensitivity. This allows us to build a model of the temperature dependence of the electrical conductivity of the sensor in a complex multicomponent gas mixture based on individual „clean“ signals obtained from the results of preliminary calibration of the sensor for each individual component of the gas mixture, taking into account cross sensitivity to other measured components of the gas mixture.

Keywords: electrical conductivity, adsorption, gas sensor, semiconductor, selectivity, regression approximation function.

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This work develops the data processing model proposed in Ref. [1] for selectively determining the concentrations of volatile organic compounds (VOCs) in ambient air. The main objective was to demonstrate, using gas mixtures with metrologically validated compositions, that the temperature response of a semiconductor resistive sensor (made of tin dioxide or tin-dioxide-based materials) to the concentration of the gas mixture under study can be approximated by the sum of the concentration responses to its individual components. The response $U_{\text{mix}}(T)$ of a semiconductor gas sensor operating in a temperature-cycling mode to a gas mixture is represented as the sum of the individual contributions $U_j(T)$ of each component j to the total detected signal (the assumption that each measured gas component contributes additively to the total sensor conductance signal is supported by the data in Ref. [2]):

$$U_{\text{mix}}(T) \approx \sum_{j=1}^{N} U_j(T), \tag{1}$$

where $U_j(T)$ is the temperature dependence of the sensor signal in the presence of gas j in the analyzed medium, and N is the number of components to be determined in the gas mixture.

With linear temperature modulation, the part of the sensor response due to gas j in the medium corresponds to its response at a certain concentration of that component in a „pure“ gas. The assumption of additive responses of gas mixture components in terms of sensor conductance is justified experimentally: within the target concentration ranges, resistive metal−oxide−semiconductor (MOS) sensors generally exhibit a linear response to the concentration of an individual gas [3]. This allows the response to a mixture to be modeled using calibration data for its individual components.

The discrimination algorithm is based on a mathematical model describing the dynamic sensor response upon exposure to a multicomponent gas mixture. Specifically, the total signal X_n is treated as the sum of the responses to individual gas components at a given temperature [2]:

$$X_n = a_{n1}s_1 + a_{n2}s_2 + \ldots + a_{nM}s_{mM}, \tag{2}$$

where X_n are the observed mixture signals, $s_1, s_2, \ldots, s_M$ are independent sources (signal amplitudes of the gas mixture components), and a_{nM} are cross-sensitivity coefficients representing the contribution of each gas to the overall response.

A „Microgas-FM12“ gas mixing system was used to obtain metrologically validated hydrogen concentrations. The concentrations were established by exponential dilution of a certified reference gas mixture [4].

Using independent component analysis, a system of linear algebraic equations (3) was constructed. Its solutions give the signals of individual components j contributing to the overall temperature dependence of the tin dioxide (SnO_2) sensor response:

$$\begin{cases} U_{\text{mix}}(T_1) = \sum_{j=1}^{N} U_j(T_1), \\ \ldots \\ U_{\text{mix}}(T_N) = \sum_{j=1}^{N} U_j(T_N). \end{cases} \tag{3}$$

For each component j, the temperature dependence of the sensor signal of interest $U_j(T)$ is measured at several known concentrations C_i (up to 5 different concentrations within the specified measurement range are necessary and sufficient). These experimental curves are generally

bell-shaped, with maximum conductance at an optimum detection temperature. For subsequent calculations, the data from „binary“ „pure“ calibrations are approximated by an analytical function of the form

$$U_j(T) = \frac{P_{m_i}}{\left[1 + \left(\frac{K_{a_i}}{T}\right)^{H_{a_i}}\right]\left[1 + \left(\frac{T}{K_{i_i}}\right)^{H_{i_i}}\right]}, \qquad (4)$$

where P_{m_i}, K_{a_i}, H_{a_i}, K_{i_i}, and H_{i_i} are the fitting coefficients for concentrations C_i $(i = 5)$ of component j of the mixture.

The sensor was calibrated over the specified concentration range using both the temperatures of the conductance extrema and the areas under the conductance curves over the specified temperature modulation interval. The known calibration concentrations of an individual component were then used to construct a system of equations, whose solution was a set of five parameters of function (4), which approximates the temperature dependence of conductance for the component concentration to be determined. The temperature at which cross-sensitivity to another component present in the gas mixture is evaluated corresponds to that component's maximum sensitivity. For example, for methane as an accompanying component, this temperature is $\sim 500\,^{\circ}\mathrm{C}$.

Each equation in system (5) represents conditions relating the parameters of the fitting function to the measured conductance at a known concentration of a gas mixture component:

$$\frac{U_j(T)}{\int\limits_{T_1}^{T_2} \frac{P_{m_A}}{\left[1+\left(\frac{K_{a_A}}{T}\right)^{H_{a_A}}\right]\left[1+\left(\frac{T}{K_{i_A}}\right)^{H_{i_A}}\right]} dT} - \frac{k(C_i)^n}{aC_A^2 + bC_A + c} = 0, \qquad (5)$$

where C_A is the known concentration for which the signal is constructed; k and n are coefficients obtained from the temperature maxima; and a, b, and c are coefficients obtained from the areas under the calibration curves. To test the discrimination algorithm, the mixture signal $U_{\mathrm{mix}}(T)$ was calculated numerically in a model experiment using the equations and measurement uncertainty calculation tables from Refs. [1,5].

Conflict of interest

The authors declare that they have no conflict of interest.

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