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Optimization of structure and power supply conditions of catalytic gas sensor

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Abstract

The analytical optimization of the structure and the power supply conditions of the catalytic gas sensor consisting of two spherical elements and connected to a Wheatstone bridge circuit is presented. Expressions for the parameters of the sensitive and reference elements and the catalytic gas sensor connected to the bridge circuit are obtained. The ratio of the sensitivity of the catalytic gas sensor to the bias voltage of the bridge circuit is chosen as a goal function and the heat balance equation for the element of the sensor in ambient air without combustible gases is used as a constraint. The diameter of the elements and the bias voltage of the bridge circuit are chosen as independent parameters. The optimization problem of the catalytic gas sensor is solved by its transformation to one parameter optimization problem without the constraint. Dependencies of optimum values of the goal function and corresponding values of the independent parameters, the sensitivity, the resistance of each element, the consumed power of each element and the current density flowing through the elements on the design parameters of the elements and their operating temperature are determined. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Analytical optimization; Catalytic gas sensor; Sensitivity of catalytic gas sensor; Combustible gas

1. Introduction

Catalytic gas sensors are widely used for measuring pre-explosive concentrations of combustible gases [1–5]. An operation principle of these sensors is based on catalytic oxidation of a combustible gas. The thermal energy that is liberated as a result of this reaction increases the temperature of a catalyst support. The change of a support temperature is determined by the concentration of the combustible gas in ambient air and is measured by a temperature sensitive element.

There is a large variety of catalytic gas sensors: from bulk sensors to microelectronics sensors made by CMOS, micromachining and thin-film technologies. However, one of widely useful structures of these sensors is the structure which contains two bead elements: sensitive and reference. Both elements consist of a platinum wire coil that is embedded in a porous refractory spherical support, usually alumina. The support of the sensitive element is doped with a catalyst chosen to suit the combustible gas to be detected. The support of the reference element has no catalyst. The sensitive and reference elements are connected to a Wheatstone bridge circuit together with two resistors having a considerably higher resistance in comparison with the resistance of these elements. Both elements are arranged in one arm of the bridge circuit and two resistors are arranged in other arm. The elements are heated to their normal operating temperature (usually, 300–600 °C) through the applied bias voltage of the bridge circuit. The bridge circuit is balanced initially in air free of a combustible gas. In the presence of a combustible gas, the resistance of the sensitive element increases and the balance of the bridge circuit is disturbed. The output signal of the bridge circuit (diagonal voltage) is changed nearly linearly with increasing concentration of a combustible gas.

In designing this catalytic gas sensor, it is important to choose such values of the design parameters and the bias voltage for which the normal operating temperature of the elements is ensured and the output signal of the bridge circuit achieves the maximum value under the given concentration of a combustible gas. This problem is the optimization problem and up to this point, it has not been considered.

This paper presents the analytical model that allows us to optimize the structure and the power supply conditions of the catalytic gas sensor with spherical elements. Furthermore, this paper considers the application of the present analytical model for the practical optimization of the catalytic gas sensor.

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2. Problem formulation

Creating an analytical optimization model of any object is a complicated problem. This problem involves some modeling levels and a optimization problem proper including the formulation of the optimization problem, the determination of a goal function and constraints, and the decision of the optimization problem. Furthermore, an analytical optimization model can be created only for an idealized object. In this connection, it is necessary to define, firstly, a number of assumptions to be used in creating the optimization model of the catalytic gas sensor and, secondly, the number of modeling levels and their content.

The present optimization model is based on the following assumptions:

1. The support of the elements has a strictly spherical shape and its shape is dependent on the parameters of a platinum wire coil: its length and external diameter. From this assumption, it follows that for the platinum wire coil, the ratio of its length to external diameter must be equal to 1. Only in this case, one can make the support whose shape is most like to spherical one. For this structure of the element, the resistance of the platinum wire coil and the diameter of the element are interdependent parameters. Therefore, for the optimization, only one of these parameters can be used as an independent parameter. Choosing the diameter of the element as the independent parameter is most acceptable since other parameters of the element are easily determined through one.
2. The catalytic oxidation rate of a combustible gas is limited by the rate of its mass transfer to the surface of the sensitive element and practically is equal to this rate. This assumption is true for the working conditions of the catalytic gas sensor (the low concentrations of a combustible gas—units vol.%; the high operating temperature of the elements—300–600 °C). For the low concentrations of a combustible gas and the high operating temperatures, round the sensitive element the layer depleted the combustible gas is formed. This is due to the fact that the processes of catalytic oxidation on the surface of this element have the higher rate than the process of the mass transfer of a combustible gas in ambient air. The thickness of the depletion layer is considerable and, therefore, the total rate of catalytic oxidation of a combustible gas is controlled by the rate of the mass transfer of a combustible gas through this layer to the surface of the sensitive element.

The modeling levels can be defined by considering the operating conditions of the catalytic gas sensor. Taking into account that, firstly, the catalytic gas sensor operates at high temperatures and, second, the concentration of a combustible gas is converted into the thermal signal by the sensitive element and then only into the output electrical signal by the bridge circuit, for creating the present optimization model, one can use two modeling levels. At the first modeling level, it is necessary to consider effects in the elements of the catalytic gas sensor and determine the parameters of these elements necessary for the further use. At the second modeling level, it is necessary to consider the catalytic gas sensor connected to the bridge circuit and determine its basic parameters. The basis of this modeling level are heat balance equations for the elements of the catalytic gas sensor connected to the bridge circuit. These equations are:

- for the sensitive element

$$\frac{U^2R_s}{(R_s+R_r)^2}+k_fk_eF\gamma Q_gC_g=h_sF(T_s-T_{en}); \tag{1}$$

- for the reference element

$$\frac{U^2R_r}{(R_s+R_r)^2}=h_rF(T_r-T_{en}), \tag{2}$$

where U is the bias voltage of the bridge circuit, R_s and R_r are the resistances of the sensitive and reference elements, respectively, k_f the mass transfer coefficient of an air filter (any catalytic gas sensor contains an air filter to protect its elements from faults), k_e the catalyst efficiency coefficient of the sensitive element, F the geometrical area of the element, i.e. $F=\pi d^2$, where d is the diameter of the element, γ the mass transfer coefficient of a combustible gas to the surface of the element, Q_g the heat of combustion of a combustible gas, C_g the volume concentration of a combustible gas in ambient air, h_s and h_r are the total heat transfer coefficients of the sensitive and reference elements, respectively, T_s, T_r and T_{en} are the absolute temperatures of the sensitive and reference elements and an environment, respectively.

The heat balance Eqs. (1) and (2) contain the parameters, which depend on the diameter of the elements and their temperatures. These parameters are R_s, R_r, h_s, h_r and γ. Thus, at the first modeling level, it is necessary to determine the dependencies of these parameters on d and T_s or T_r.

3. Parameters of the sensitive and reference elements

The catalytic gas sensor under consideration contains two elements: sensitive and reference, which have the identical structure from the point of view of their design dimensions. The typical structure of the element is shown in Fig. 1. Taking into account the identical structure of both elements the determination of the expressions for their parameters will be carried out for one element (e.g. sensitive element). These parameters will be marked with sub-index ''el''.

3.1. Expression for the resistance of the elements

The temperature dependence of the element resistance is defined by the following well known expression:

$$R_{el}=R_0[1+\alpha(T_{el}-T_0)], \tag{3}$$

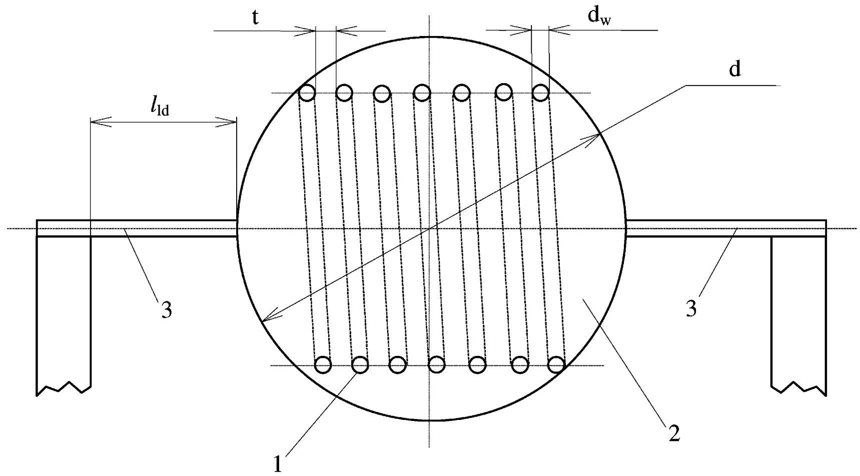

Fig. 1. Structure of the element of the catalytic gas sensor: (1) platinum wire coil, (2) support, (3) lead of the element, (t) distance between the turns of the coil, (d_w) diameter of the platinum wire, (d) diameter of the element, (l_{ld}) length of the lead.

where R_{el} and R_0 are the resistances of the element at temperatures T_{el} and T_0, respectively, α is the temperature resistance coefficient of the wire coil material, T_{el} the operating temperature of the element, $T_0 = 273.15$ K the absolute temperature corresponding 0 °C.

The dependence of R_0 on the diameter of the element d was obtained from analysis of the element structure shown in Fig. 1 and can be presented as follows:

$$R_0 = 2\rho_0 d \frac{\sqrt{[\pi(d - (8)^{0.5} d_w)]^2 + 2(d_w + t)^2}}{\pi d_w^2 (d_w + t)}, \quad (4)$$

where ρ_0 is the volume resistivity of the wire coil material at T_0, d_w the diameter of the wire used in the coil, t the distance between turns of the wire coil.

3.2. Expression for the total heat transfer coefficient of the elements

The thermal power generated by the elements of the catalytic gas sensor as a result of electrical current flow through ones and catalytic oxidation of a combustible gas on the surface of the sensitive element is basically dissipated by three ways: the free convection heat transfer, the radiant heat transfer from the element and the heat transfer through element leads. In this case, the expression for the total heat transfer coefficient of the element h_{el} can be written as follows:

$$h_{el} = h_{fc} + h_{rad} + h_{ld}, \quad (5)$$

where h_{fc} is the free convection heat transfer coefficient of the element, h_{rad} the radiant heat transfer coefficient of the element, h_{ld} the heat transfer coefficient through the element leads.

The expression for h_{fc} can be found by using the similarity theory [6]. According to this theory, the free convection heat transfer coefficient can be presented as follows:

$$h_{fc} = \frac{Nu\lambda}{d}, \quad (6)$$

where Nu is the Nusselt number, λ the thermal conductivity of ambient air.

For a free convection heat transfer from a spherical body, the Nusselt number can be written in the following form [6]:

$$Nu = 2 + 0.5(Gr\,Pr)^{0.25}, \quad (7)$$

where Gr is the Grashof number, Pr the Prandtl number.

The Grashof number and the Prandtl number are determined as follows:

$$Gr = \frac{\beta g d^3 (T_{el} - T_{en})}{v^2}; \quad (8)$$

$$Pr = \frac{v}{a}, \quad (9)$$

where β is the thermal coefficient of volumetric expansion of ambient air, g the gravity acceleration, v the kinematic viscosity of ambient air, a the thermal diffusivity of ambient air:

$$a = \frac{\lambda}{c_p \rho}, \quad (10)$$

where c_p is the specific heat of ambient air at constant pressure, ρ the ambient air density.

The ambient air parameters λ, v, c_p, and ρ in the Eqs. (6), (8)–(10) are the temperature dependence parameters. Their temperature dependencies and the value of the thermal coefficient of volumetric expansion are given in Appendix A.

Thus, using Eqs. (7)–(9), Eq. (6) for h_{fc} can be rewritten as follows:

$$h_{fc} = \frac{2\lambda}{d} + 0.5\lambda \left[\frac{\beta g (T_{el} - T_{en})}{dva}\right]^{0.25}. \quad (11)$$

The radiant heat transfer coefficient of the element can be determined from the expression for the power of the radiant heat transfer P_{rad}:

$$P_{rad} = \varepsilon_{el}\sigma_b F(T_{el}^4 - T_{en}^4) = \varepsilon_{el}\sigma_b F(T_{el}^2 + T_{en}^2)(T_{el} + T_{en})(T_{el} - T_{en}), \quad (12)$$

where ε_{el} is the emissivity of the element, σ_b the Stefan–Boltzmann constant. On the basis of Eq. (12), one can write the expression for h_{rad}:

$$h_{rad} = \varepsilon_{el}\sigma_b(T_{el}^2 + T_{en}^2)(T_{el} + T_{en}). \quad (13)$$

The heat transfer coefficient through the element leads takes into account the convective and radiant heat transfer and the heat transfer by means of the thermal conduction. To use the heat transfer coefficient through the element leads in Eq. (5), this coefficient has to be normalized by the geometrical area of the element. The expression for h_{ld} was obtained in [7] and can be written as follows:

$$h_{ld} = \frac{\pi d_w^2 \lambda_w m \coth(m l_{ld})}{2\pi d^2}, \quad (14)$$

where

$$m = 2\sqrt{\frac{(\lambda/2d_w) + \varepsilon_w\sigma_b(T_{ld}^2 + T_{en}^2)(T_{ld} + T_{en})}{d_w\lambda_w}}, \quad (15)$$

$$T_{ld} = \frac{T_{el} + T_{en}}{2}, \quad (16)$$

where λ_w and ε_w are the thermal conductivity and the emissivity of the leads material, respectively, l_{ld} is the length of the element lead.

Using Eqs. (11), (13) and (14), the final expression for the total heat transfer coefficient of the element can be represented as follows:

$$h_{el} = \frac{2\lambda}{d} + 0.5\lambda\left[\frac{\beta g(T_{el} - T_{en})}{d\nu a}\right]^{0.25} + \varepsilon_{el}\sigma_b(T_{el}^2 + T_{en}^2)(T_{el} + T_{en}) + \frac{\pi d_w^2 \lambda_w m \coth(m l_{ld})}{2\pi d^2}. \quad (17)$$

3.3. Expression for the mass transfer coefficient of a combustible gas

The combustible gas transfer to the surface of the sensitive element is realized by means of free convection and diffusion. The first mechanism is due to temperature difference between the element and ambient air and the second mechanism is due to concentration difference of a combustible gas on the surface of the element and in ambient air. The first mechanism is prevalent since the temperature difference is considerable (hundreds of degrees). In one's turn, the second mechanism can be disregarded since the concentration difference do not exceed units vol.% and, therefore, its influence on the combustible gas transfer to the surface of the element is far less than the free convection influence. Thus, in obtaining the expression for the mass transfer coefficient of a combustible gas, one can take into account only the transfer of this gas by means of free convection.

The expression for the mass transfer coefficient γ is defined as well as for h_{fc} by using the similarity theory. According to [6], one can write the following expression for γ:

$$\gamma = \frac{ShD}{d}, \quad (18)$$

where Sh is the Sherwood number, D the diffusivity of a combustible gas in ambient air. The temperature dependencies of the diffusivity for a number of combustible gases are given in Appendix A.

Taking into account that, firstly, the free convection is prevalent mechanism of the combustible gas transfer to the surface of the sensitive element and, secondly, for the normal conditions, the Prandtl number is approximately equal to the Schmidt number, the Sherwood number can be represented as follows [6]:

$$Sh = 2 + 0.5(Gr\,Sc)^{0.25}, \quad (19)$$

where Sc is the Schmidt number.

The Schmidt number is

$$Sc = \frac{\nu}{D}. \quad (20)$$

Using Eqs. (8), (19) and (20), Eq. (18) for γ can be rewritten as follows:

$$\gamma = \frac{2D}{d} + 0.5D\left[\frac{\beta g(T_{el} - T_{en})}{d\nu D}\right]^{0.25}. \quad (21)$$

Thus, in the present part, all parameters which characterize each element have been determined and one can consider parameters of the catalytic gas sensor connected to the bridge circuit.

4. Parameters of the catalytic gas sensor connected to the bridge circuit

The catalytic gas sensor is connected to the bridge circuit as shown in Fig. 2. A basic parameter of the catalytic gas sensor is the sensitivity to the concentration of a combustible gas.

4.1. The sensitivity of the catalytic gas sensor to the concentration of a combustible gas

The sensitivity of the catalytic gas sensor to the concentration of a combustible gas S is defined as follows:

$$S = \frac{U_{out}}{C_g}, \quad (22)$$

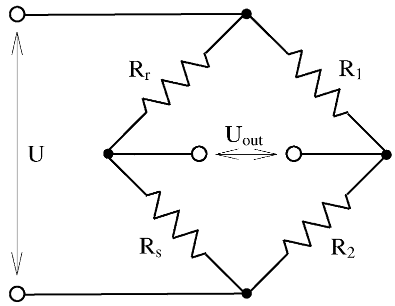

Fig. 2. Bridge circuit of connection of the catalytic gas sensor: (U) bias voltage, (U_{out}) output voltage of the bridge circuit, (R_r) reference element of the catalytic gas sensor, (R_s) sensitive element of the catalytic gas sensor, (R_1, R_2) resistors.

where U_{out} is the output diagonal voltage of the bridge circuit. For $R_1=R_2$, the output diagonal voltage of the bridge circuit is given as

$$U_{out} = \frac{U(R_s - R_r)}{2(R_s + R_r)}. \tag{23}$$

Taking into account Eq. (3) for the resistance of the sensitive and reference elements and Eq. (23), the expression for the sensitivity of the catalytic gas sensor can be represented as follows:

$$S = \frac{U\alpha(T_s - T_r)}{2C_g[2 + \alpha(T_s + T_r - 2T_0)]}. \tag{24}$$

As can be seen from the Eq. (24), the sensitivity of the catalytic gas sensor depends on the bias voltage of the bridge circuit and the temperatures of its elements. In its turn, the temperatures of the elements are determined by the bias voltage, the design parameters of the elements and the ambient air parameters. Therefore, determining the temperatures of the elements is the basic problem for considering the catalytic gas sensor connected to the bridge circuit.

4.2. Temperatures of the elements of the catalytic gas sensor connected to the bridge circuit

The temperatures of the elements can be determined by means of solving the system of the heat balance equations for the catalytic gas sensor connected to the bridge circuit. This system consists of Eqs. (1) and (2). As demonstrated above, in these equations, parameters R_s, R_r, h_s, h_r and γ are temperature dependence parameters. Moreover, the temperature dependencies of h_s, h_r and γ are very complicated. Therefore, an analytical solution of this system concerning temperatures T_s and T_r is impossible. However, this system can be transformed by expressing one independence parameter through the other and its solution can be reduced to numerical solution of one equation with one independence parameter.

Substituting into Eqs. (1) and (2), the temperature dependencies of R_s and R_r according to Eq. (3) and transforming these equations yield the following system of the equations:

$$\frac{U^2}{R_0[2+\alpha(T_s+T_r-2T_0)]^2} = \frac{\pi d^2[h_s(T_s - T_{en}) - k_f k_e \gamma Q_g C_g]}{1 + \alpha(T_s - T_0)}; \tag{25}$$

$$\frac{U^2}{R_0[2 + \alpha(T_s + T_r - 2T_0)]^2} = \frac{\pi d^2 h_r(T_r - T_{en})}{1 + \alpha(T_r - T_0)}. \tag{26}$$

From Eq. (25), the temperature of the reference element, T_r, can be presented as a function of T_s:

$$T_r = \frac{U}{\alpha}\left(\frac{1+\alpha(T_s - T_0)}{\pi d^2 R_0[h_s(T_s - T_{en}) - k_f k_e \gamma Q_g C_g]}\right)^{0.5} - \frac{2}{\alpha} - T_s + 2T_0 \tag{27}$$

Eq. (27) contains the temperature dependence parameters h_s and γ which depend on only T_s.

Using Eq. (27) in Eq. (26) yields the equation concerning one independence parameter T_s. In this equation, the temperature dependence parameters h_s, h_r and γ are functions of T_s. The solution of this equation concerning T_s can be carried out by a numerical method. After determining the value of T_s which satisfies Eq. (26), the value of T_r is found by using Eq. (27).

5. Optimization model

The optimization aim of the catalytic gas sensor is to obtain the values of independent parameters (e.g. the design parameters of the elements, the parameters of bridge circuit) for which one of its basic output parameters attains the limiting value. In present case, the sensitivity of the catalytic gas sensor to the concentration of a combustible gas is the basic output parameter. However, as can be seen from Eq. (24), the sensitivity to a greater degree depends on the bias voltage than on the temperatures of the elements. Our investigation shows (Section 6) that this parameter increases practically linearly with increasing the bias voltage. However, the increase of the sensitivity by means of increasing the bias voltage is possible within reasonable limits. Firstly, with increasing the bias voltage, it is necessary to increase the sizes of the elements, for their operating temperature to keep. Secondly, with increasing the bias voltage, the consumed power of the sensor increases. Thirdly, the sensor will not be used in the optimum conditions since the most part of the consumed power will be dissipated in an environment, i.e. the heat loss of the sensor increases.

In this connection, for the optimization of the catalytic gas sensor, it is necessary to choose other parameter as the goal function. This parameter have to be connected with the sensitivity, but one does not have to contain the bias voltage in the evident form. One of such parameters is the ratio of the sensitivity to the bias voltage:

$$Z = \frac{S}{U} = \frac{\alpha(T_s - T_r)}{2C_g[2 + \alpha(T_s + T_r - 2T_0)]}. \quad (28)$$

Therefore, this parameter can be chosen as the goal function. In this case, the diameter of the elements and the bias voltage of the bridge circuit can be chosen as independent parameters.

For operating the catalytic gas sensor in ambient air without a combustible gas, the certain temperature of its elements have to be ensured. This temperature is called the operating temperature and its value is defined by the combustible gas to be detected and the composition of a catalyst. On the other hand, the operating temperature depends on the bias voltage of the bridge circuit, the design parameters of the elements and the ambient air parameters. Therefore, the expression which connects the operating temperature of the element in ambient air without a combustible gas, the bias voltage of the bridge circuit, the design parameters of the element, and the ambient air parameters can be used as a constraint. In our case, such an expression is the heat balance equation for the element of the catalytic gas sensor operating in ambient air without a combustible gas. Assuming that, in this atmosphere, the parameters of the elements must be identical one can write the heat balance equation for one of the elements:

$$\frac{U^2}{4R_0\left[1 + \alpha(T_{op} - T_0)\right]} = \pi d^2 h_{op}(T_{op} - T_{en}), \quad (29)$$

where T_{op} is the operating temperature of the elements in ambient air without a combustible gas, h_{op} the total heat transfer coefficient of the element at the temperature T_{op}. In the present optimization model, we shall relate the operating parameters of the element (T_{op}, h_{op}) to the sensitive element.To use Eq. (29) as the constraint this equation must be transformed to the following form:

$$U^2 - 4\pi d^2 R_0 h_{op}[1 + \alpha(T_{op} - T_0)](T_{op} - T_{en}) = 0. \quad (30)$$

Thus, the basic elements of the analytical optimization model for the catalytic gas sensor are defined. It is necessary to choose the method for its solution. In general, this problem can be decided by the method of Lagrange multipliers [8]. However, taking into account that one of two independent parameters (the bias voltage, U) is easily defined through other independent parameter (the diameter of the element, d) from the expression used as the constraint, the present optimization problem can be reduced to one parameter optimization problem without the constraint. With this end in view one must define the dependence of the bias voltage on the diameter of the element from Eq. (30). This dependence is given as

$$U = 2d\sqrt{\pi R_0 h_{op}[1 + \alpha(T_{op} - T_0)](T_{op} - T_{en})}. \quad (31)$$

In this case, only the diameter of the element remains the independent parameter and the optimization problem for the catalytic gas sensor is solved by a numerical differentiation of the goal function Z (Eq. (28)) with respect to the diameter of the element d. A maximum value of Z corresponds to the value of d for which $\partial Z/\partial d$ is equal to 0. This value of d is used to find the value of the bias voltage which as well corresponds to the maximum of the goal function.

6. Numerical results

The present model was applied for the optimization of the catalytic gas sensor with the sensitive and reference elements based on a platinum wire coil. Platinum has the following parameters: the volume resistivity $\rho_0 = 9.81 \times 10^{-8}\,\Omega\,\mathrm{m}$ at $T_0 = 273.15\,\mathrm{K}$; the temperature resistance coefficient $\alpha = 0.00396\,\mathrm{K}^{-1}$; the thermal conductivity $\lambda_w = 72.0\,\mathrm{W/(m\,K)}$; the emissivity $\varepsilon_w = 0.9$. Alumina was used as the catalyst support. The emissivity of alumina is 0.5. The mixture of platinum and palladium was chosen as the catalyst. The environment temperature T_{en} was assumed to be 300 K. The concentration of a combustible gas (methane) was equal to 1.0 vol.%. The heat of combustion of methane is 40.469 kJ/m^3. The other parameters had the following values: $k_f = 1$, $k_e = 0.2$.

Fig. 3 shows the typical dependencies of the goal function Z and the sensitivity S on the diameter of the elements and the bias voltage of the bridge circuit. These dependencies were obtained while the constraint on the operating temperature is fulfilled, i.e. other independent parameter (the bias voltage for Fig. 3a and the diameter of the elements for

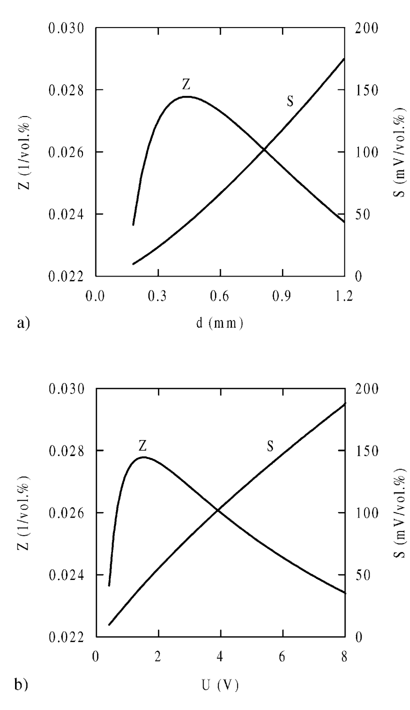

Fig. 3. Optimum values of the goal function Z and corresponding values of the sensitivity S vs. (a) diameter of the element d and (b) bias voltage of the bridge circuit U, $d_w = 20\,\mu\mathrm{m}$, $t = 20\,\mu\mathrm{m}$, $T_{op} = 450\,^{\circ}\mathrm{C}$.

Fig. 3b) was changed in accordance with the given constraint. Both dependencies of the goal function Z have a maximum while both dependencies of the sensitivity S monotonously increase with increasing the diameter of the element and the bias voltage. This fact indicates that the sensitivity can not be used as the goal function for the optimization of the catalytic gas sensor under the constraint on the operating temperature of the elements and with the given independent parameters.

The dependencies of the optimum values of the goal function Z and corresponding values of the sensitivity S, the diameter of the element d, the bias voltage of the bridge circuit U, the resistance of each element R_0, the consumed power of each element P_{op}, and the current density flowing through the elements J on the diameter of the wire used in coil d_w are shown in Fig. 4. At this point, the values of R_0 were defined by using Eq. (4) and the values of P_{op} and J were defined as follows:

$$P_{op} = \frac{U^2}{4R_0[1 + \alpha(T_{op} - T_0)]}; \quad (32)$$

$$J = \frac{2U}{\pi d_w^2 R_0[1 + \alpha(T_{op} - T_0)]}. \quad (33)$$

With increasing d_w, the optimum values of the goal function Z and the corresponding values of S, U, R_0, and J decrease. The values of d and P_{op} corresponding the optimum values of the goal function Z increase with increasing d_w.

Fig. 5 shows the dependencies of the optimum values of the goal function Z and corresponding values of the sensitivity S, the diameter of the element d, the bias voltage of the bridge circuit U, the resistance of each element R_0, the consumed power of each element P_{op}, and the current density flowing through the elements J on the distance between the turns of the coil t. The features of the dependencies is that the optimum values of the goal function Z and the corresponding values of d and P_{op} are independent on the distance between the turns of the coil. The corresponding values of S, U, R_0 decrease and the corresponding values of J increase with increasing the distance between the turns of the coil.

The dependencies of the optimum values of the goal function Z and corresponding values of the sensitivity S, the diameter of the element d, the bias voltage of the bridge circuit U, the resistance of each element R_0, the consumed power of each element P_{op}, and the current density flowing through the elements J on the operating temperature T_{op} of the elements in ambient air without the combustible gas are shown in Fig. 6. With increasing T_{op} the values of Z, S, d, U, and R_0 decrease and the values of P_{op} and J increase.

On the grounds of the data given in Figs. 4–6, it is necessary to make the following remark concerning the current density flowing through the elements of the catalytic gas sensor. In fact, in the present optimization model, it should be introduced the additional constraint on the current density flowing through the elements since its values do not have to exceed a permissible current density. For example, for the platinum wire, the permissible current density is approximately equal to 500 A/mm^2. In this connection, the values of parameters d_w, t, T_{op} for which the current density flowing through the elements is more than 500 A/mm^2 is not admissible for the given sensor structure. However,

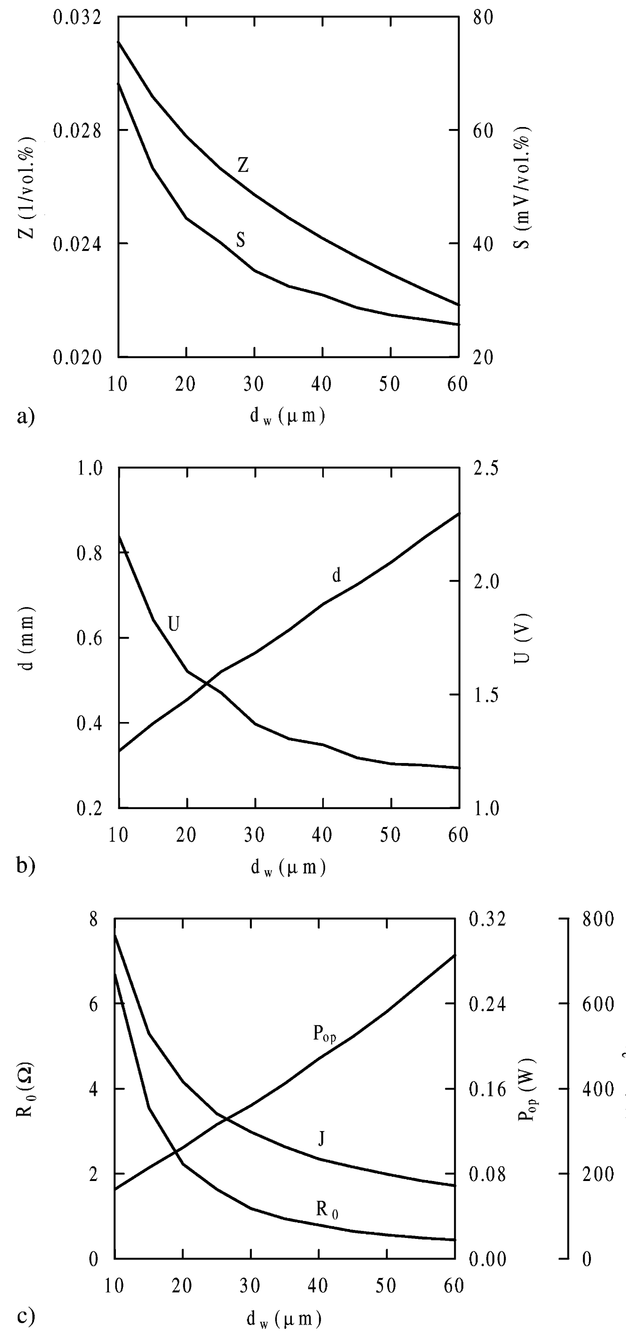

Fig. 4. Optimum values of (a) the goal function Z and corresponding values of the sensitivity S, (b) the diameter of the element d, the bias voltage of the bridge circuit U, (c) the resistance of each element R_0, the consumed power of each element P_{op}, and the current density flowing through the elements J vs. diameter of the platinum wire d_w, $t = 20$ μm, $T_{op} = 450$ °C.

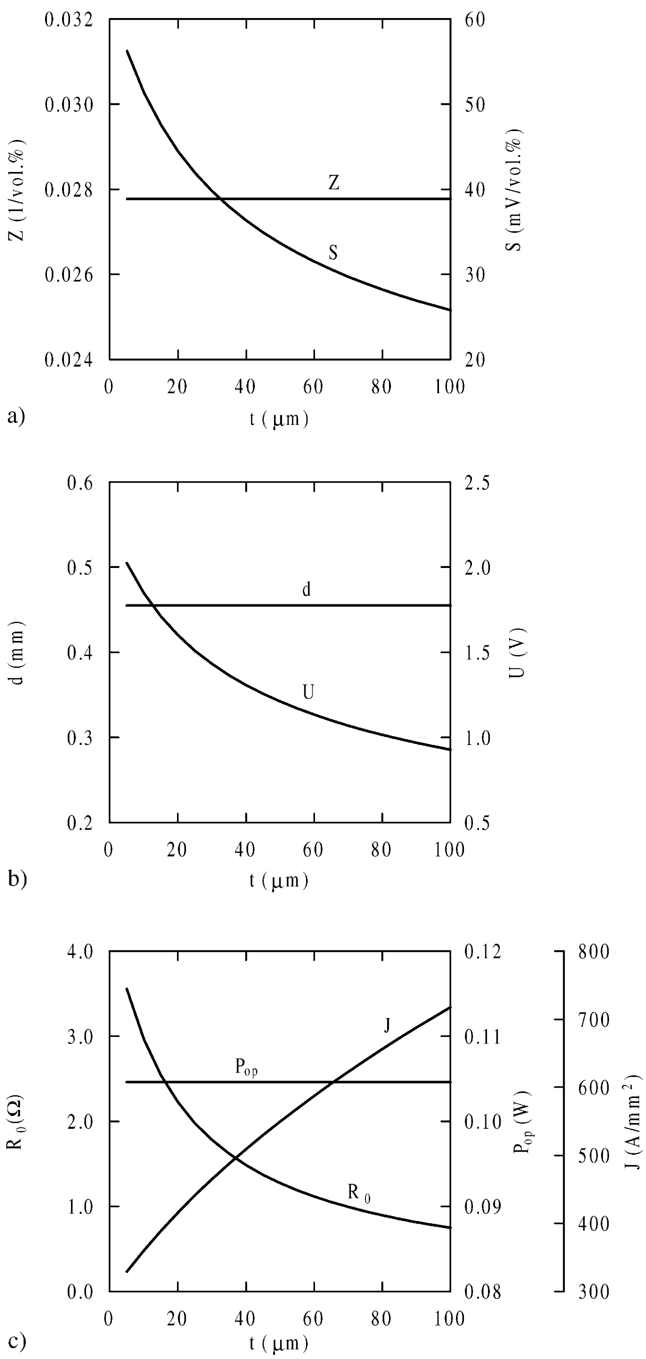

Fig. 5. Optimum values of (a) the goal function Z and corresponding values of the sensitivity S, (b) the diameter of the element d, the bias voltage of the bridge circuit U, (c) the resistance of each element R_0, the consumed power of each element P_{op}, and the current density flowing through the elements J vs. distance between turns of the platinum wire coil t, $d_w = 20$ μm, $T_{op} = 450$ °C.

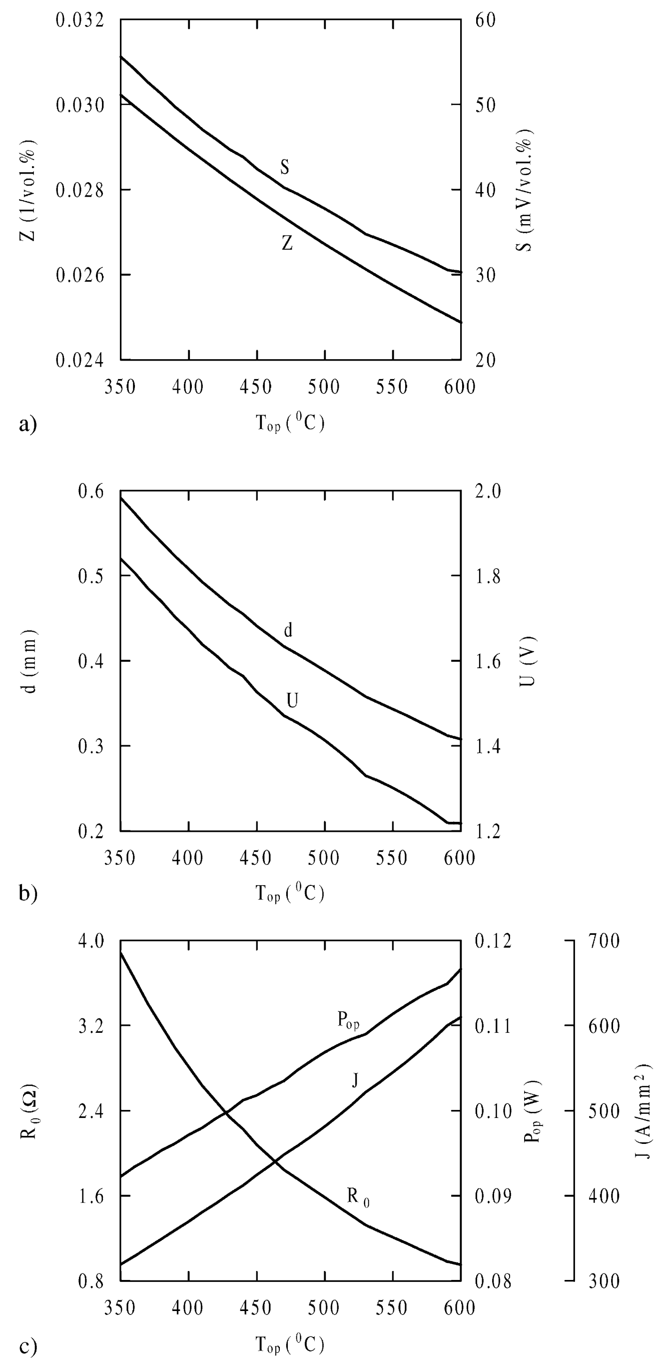

Fig. 6. Optimum values of (a) the goal function Z and corresponding values of the sensitivity S, (b) the diameter of the element d, bias voltage of the bridge circuit U, (c) the resistance of each element R_0, the consumed power of each element P_{op}, and the current density flowing through the elements J vs. operating temperature of the element T_{op}, $d_w = 20$ μm, $t = 20$ μm.

introduction of the constraint on the current density flowing through the elements in the present optimization model will vastly complicate its decision. Therefore, for using this optimization model, one can recommend to compare the obtained current density with the permissible one. If the current density flowing through the elements exceeds the permissible current density, it is necessary to change the given values of their design parameters: to increase the diameter of the platinum wire and/or to decrease the distance between turns of the platinum wire coil.

7. Conclusion

The present analytical optimization model of the catalytic gas sensor connected to the bridge circuit permits the diameter of the elements and the bias voltage of the bridge circuit for which the maximum ratio of the sensitivity to the bias voltage is assured under the given operating temperature, to be obtained.

This model can be also applied for the optimization of the catalytic gas sensors in which the elements have the shape similar to the spherical one (e.g. the ellipsoid of rotation). In this case, one can use the assumption about the negligible distinction between the conditions of the heat and mass transfers for these elements and the spherical element. Incidentally, the mathematical expressions are not changed since, in the optimization model, one can use the average diameter of the non-spherical element instead of the diameter of the spherical element. However, for creating the optimization model, it is necessary to determine a relation between the resistance of the platinum wire coil and the average diameter of the non-spherical element.

Using this optimization model for other catalytic gas sensors (e.g. the sensors made by CMOS, micromachining and thin-film technologies) demands to determine the dependencies of the heat and mass transfer coefficients on the dimensions and the temperature of a substrate on which the catalytic layer and the element performing simultaneously functions of a heater and a temperature sensitive element are placed. Furthermore, it is necessary to determine a relation between design parameters of the mentioned element and the catalytic layer, on the one hand, and the dimensions of a substrate, on the other hand.

In addition, the present optimization model can be used in CAD tools for the catalytic gas sensors as a component of these tools.

Appendix A

The elements of the catalytic gas sensor usually operate in ambient air that has the following features. Firstly, the ambient air temperature is changed in the normal to the surface of the element from the maximum value corresponding the temperature of the element to the minimum value corresponding an environment temperature at a considerable distance from the element. Secondly, for operating the catalytic gas sensor, ambient air is the air with a small addition of a combustible gas (units vol.%). Taking into account these features, for determining the temperature dependencies of the ambient air parameters, the following assumptions are used:

1. The ambient air temperature T_a around the elements is assumed to be equal to the average temperature between the maximum and minimum values, i.e. between the temperature of the element T_{el} and the environment temperature T_{en}

$$T_a = \frac{T_{el} + T_{en}}{2}.$$

2. The ambient air parameters are assumed to be equal to the uncontaminated air parameters. The small addition of a combustible gas is not taken into account since this addition has a negligible influence on the ambient air parameters.

The analytical temperature dependencies of the ambient air parameters (ρ, the density; λ, the thermal conductivity; c_p, the specific heat at constant pressure; ν, the kinematic viscosity) are determined by means of an approximation of experimental temperature dependencies for the uncontaminated air in temperature interval 300–1000 K. The experimental temperature dependencies of the uncontaminated air parameters are given in [9]. In present optimization model, they are approximated by the third power polynomial

$$b = b_0 + b_1 T_a + b_2 T_a^2 + b_3 T_a^3,$$

where b is the ambient air parameter, b_0, b_1, b_2, b_3 are the polynomial coefficients. The values of the polynomial coefficients have been determined by the least squares method and are given in the Table 1.

Taking into account the second assumption, in the present optimization model, use is made of the thermal coefficient of volumetric expansion for the uncontaminated air equal to $3.665 \times 10^{-3}\ \text{K}^{-1}$.

The temperature dependence of the diffusivity of a combustible gas in the air is determined by using the following expression [10]:

$$D = D_0 \left(\frac{T_a}{T_0}\right)^{\alpha},$$

Table 1
The values of the polynomial coefficients for the ambient air parameters

Parameter	Polynomial coefficients			
	b_0	b_1	b_2	b_3
ρ	2.62483	-6.90019×10^{-3}	7.62042×10^{-6}	-3.00127×10^{-9}
λ	-1.33351×10^{-4}	1.00151×10^{-4}	-4.40284×10^{-8}	1.15754×10^{-11}
c_p	1034.5	-2.82248×10^{-1}	7.08857×10^{-4}	-3.19875×10^{-7}
ν	1.62841×10^{-6}	2.75665×10^{-9}	1.61342×10^{-10}	-4.83107×10^{-14}

where D_0 is the diffusivity of a combustible gas in the normal conditions (pressure, -101325 Pa; temperature, -273.15 K), $T_0 = 273.15$ K, α the coefficient. The values of D_0 and α for a number of combustible gases are given in [10].

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Biography

Alexander G. Kozlov was born in Omsk, Russia, in 1955. He received the diploma in engineering in radioelectronics from the Technical Institute of Omsk in 1977 and the PhD degree in microelectronics from the Electrotechnical Institute of St. Petersburg, Russia, in 1984. From 1977 to 1981 and from 1985 to 1991, he was with the Technical Institute of Omsk working in consecutive order assistant lecturer, lecturer and reader. From 1981 to 1984, he was doctoral student in the Electrotechnical Institute of St. Petersburg, Russia. In 1992, he joined the Institute of Sensor Microelectronics RAS where since 1995, he has been a head of laboratory. His current research interests are solid state gas sensors, simulation and optimization of semiconductor and thin-film sensors.