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Numerical simulation of IR MEMS thermopile sensors

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Abstract

The main parameters of TPA IR sensors were calculated using analytical relations and finite element simulation. The simulation was performed using the software packages ANSYS and Synopsys TCAD to determine possible limiting characteristics of the sensor and to optimize its design. The paper presents the simulation results of thermo-mechanical deformations occurring in the structure of the sensor as a result of the high temperature processes in the manufacture of the sensing element, the response dynamic of the sensor to thermal radiation and 2D temperature maps in the state of thermal equilibrium with an external heat picture. We obtained the main sensitivity parameters of the considered MEMS sensors structures using the data of simulation. For sensor with single thermocouple volt-watt sensitivity $\Delta V/\Delta P \approx 620$ V/W, noise equivalent temperature difference in the object of observation (τ_f=0,1s) NETD ≈ 28,7 mK and for sensor with two thermocouples – volt-watt sensitivity $\Delta V/\Delta P = 455$ V/W, noise equivalent temperature difference in the object of observation (τ_f=0,1s) NETD ≈ 38.4 mK. The obtained results allowed to optimize the IR TPA design.

Keywords: infrared (IR), microelectromechanical systems MEMS), CMOS, membrane, noise equivalent temperature difference (NETD), sensor, thermopile array (TPA).

Introduction

The use of IR FPA in any potential area of application is primarily based on, along with their sensitivity, cost, power consumption and weight. Attach importance to the reliability and ease of use too. Uncooled IR FPA actively developed the last three decades satisfy all these requirements. Currently, the bolometric FPA are of greatest use (FPA of 2048 x 1536 format [1] are available and their parameters are close to the cryogenic arrays).

The competitive trend in the development of uncooled thermal receivers are multi-element heat arrays with the thermocouples sensitive elements [2]. Wide operation temperature range, no need of temperature stabilization, and radiometric accuracy of thermocouples makes them attractive in the future to create compact and cheap imaging system with low power consumption. This opens up the possibility of their wide use in the whole range of civilian applications [3]. Moreover, the major advantage of thermocouple IR sensors is the compatibility of technological processes of sensors fabrication with standard CMOS technology.

Current level of this field development is characterized, for example, a commercial line of opto-electronic modules with a TPA of 8x8, 32x32, 64x64 and 82x62 formats of the Heimann Sensor GmbH company [4]. Japan Defence Agency and NEC Corporation in 1994 announced making of a thermocouple matrix with number of elements 128x128 [5]. In [6] (Nissan Research Center) the results of TPA of 120x90 format development are presented. The state and prospects of development IR FPA with thermocouple transducers of thermal radiation were considered in [7]. It should be noted that the number of publications on this subject is very limited.

Object and methodology of modeling

When designing IR TPA it is necessary to take into account many parameters in order to establish patterns of functioning or to design a sensor with desired or optimum characteristics. Because of the small sensor size the influence of different background (parasitic) impacts on its functioning increases. The influence of some of them can be evaluated analytically. First of all, it concerns the processes of heat transfer and the formation of the output electrical signal [8, 9].

It is very difficult or even impossible to analytically evaluate the other part of them, namely mechanical deformation and stresses in the sensor mount consoles, because of the many layers and well-developed 3-dimensional geometry. In addition, although non-stationary thermal processes in the sensor can be theoretically estimated, the question remains about the accuracy of these estimates. Therefore, it is necessary to resort to numerical modeling and choose the most acceptable sensor design using simulation results.

The investigated sensor (Fig. 1) is a structure consisting of a dielectric (SiO_2) membrane with heat-absorbing layer (Si_3N_4) on which "hot" junctions of thermocouples with shoulders of polycrystalline silicon p-Si* and n-Si* are located. The membrane is suspended with the help of the poorly heat-conductive load-bearing consoles of SiO_2, on which the shoulders of the thermocouples are located. "Cold" contacts of the thermocouples are located on a silicon substrate which plays the role of a tank with a constant temperature Thermocouples connected in series on the side of "cold" contacts.

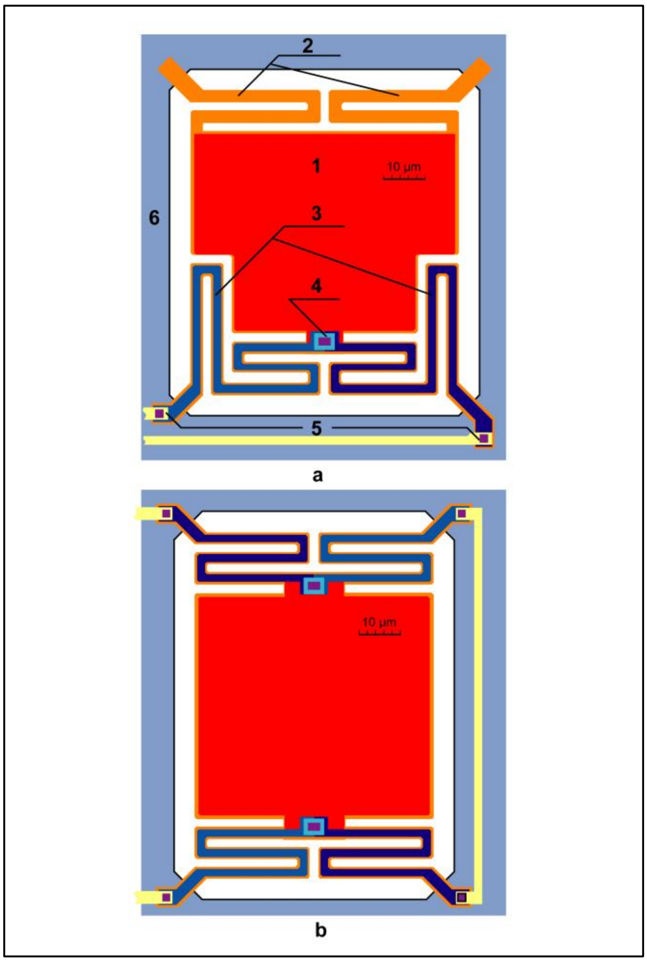


Fig. 1. Sensor topology versions: a – one thermocouple, b – two thermocouples
1 – membrane with the absorbing layer, 2 – free console, 3 – console with thermocouple, 4 – «hot» seal of the thermocouple, 5 – "cold" contacts of the thermocouples, 6 – substrate.

Sensor layout was generated using 1.2 µm design rule of standard CMOS technology. In addition, for layout generation the results of the theoretical analysis [12, 13] were used. It allowed to optimize the geometrical parameters of the elements included in the sensor, namely the thickness and length of the thermocouples, heat sensitive membrane area and the total (averaged) thickness of the membrane. In these calculations the noise equivalent temperature difference (NETD) was used as a parameter that determines the quality of the sensor, i.e., we have taken as the optimal geometrical and technological parameters such that minimize NETD.

Topological dimensions of the sensor are optimized in a similar way. Topology with one thermocouple (Fig.1a) is characterized by the following values: surface area of the absorbing IR-radiation region of the membrane $A = 2{,}8 \bullet 10^{-5}$ cm^2, the area occupied by consoles thermocouple $A_c = 1{,}4 \bullet 10^{-5}$ cm^2. The two thermocouples sensor dimentions (Fig.1b) are $A = 3{,}3 \bullet 10^{-5}$cм^2 and $A_c = 1{,}7 \bullet 10^{-5}$ cm^2. Console width for both types of sensors is equal to 3 µm, and the width of thermocouples – 2 µm.

The simulation was performed using the software packages ANSYS and Synopsys TCAD to determine possible limiting characteristics of the sensor and verify the theoretical calculations. Thermo-mechanical deformations occurring in the structure of the sensor as a result of the high temperature processes in the sensor manufacturing, the dynamic response of the sensor to thermal radiation and 2D temperature maps in the state of thermal equilibrium with an external heat stage were studied. Numerical values of the material parameters of the sensor used in the simulation are presented in table 1.

A. Modeling of deformation

The technological process of manufacturing of IR FPA with thermocouple sensors integrated with CMOS circuits includes high temperature (up to 500C) operations. The formation of the sensor layers with different thermomechanical parameters at these temperatures and the subsequent cooling may cause deformation, affecting the performance of the sensor. Thermal isolation of the sensitive membrane of the sensor is provided by a spatial gap between it and the substrate, formed by etching of the layer under the membrane or the through well in the substrate. The membrane is mechanically connected to the substrate by only a narrow poorly heat conductive consoles. Thus, the membrane consisting of films with submicron and micron thicknesses, in fact, freely placed in space and occurring layer stresses lead to deformations which is not compensated by the array substrate. Modeling of these deformations gives the possibility to consider and reduce their negative influence on the performance of the sensor in its design.

Table 1.

	Thickness, ***h***, µm	Density, ***ρ***x10^{-3}, kg/m^3	Young modulus, ***E***, gN/m^2	Poisson coefficient, ***ν***	Extensions coefficient, **β**x10^{-6}, K^{-1}	Thermal conductivity ***G***, W/mK	Heat capacity ***c***, J/kgK	Seebeck coefficient ***α***, µV/K
SiO_2	0,9	2,19	75	0,17	0,5	1,0	745	-
Si_3N_4	0,6	2,40	180	0,27	0,8	20	691	-
n-Si*	0,45	2,1	169	0,22	9,4	33,1	700	–140
p-Si*						30,6		160
Al	0,45	2,7	80	0,17	23,6	237	908	–1,7

B. Simulation of transient heat transfer process

Thermal microsensors is a large group of microelectronic sensors, which is characterized by the fact that thermal processes play the essential role in its functioning. Basic elements of thermal microsensors are arranged on a thin thermally isolated structure obtained by anisotropic etching of silicon or by etching the sacrificial dielectric layer. Thermocouple sensor just relates to devices of that class. Due to the good thermal insulation and low thermal mass of the membrane it is possible to create multi-element uncooled IR receivers with high sensitivity, linearity conversion, low power consumption and high speed of response to thermal effects. Nonstationary conditions play an important role in the work of the sensor. It is necessary to know sensor frequency response to define the behavior of the sensor during transient modes. Due to the great inertia of thermal processes in comparison with electric processes, the frequency response of a thermocouple sensor is mainly determined by the thermal subsystem. Therefore, the frequency characteristic can be obtained by considering non-stationary processes in its thermal subsystem.

The sensitivity of the sensor depends on the possibility of achieving maximum thermopower between the hot and cold contacts of the thermocouples over a finite time interval (it is limited by frame rate of the IR receiver) and a minimum level of thermal noise of the thermocouple, as determined by its electric resistance [12, 13]. Two processes, the absorption of heat by membrane and its transfer to the substrate by thermocouple consoles, influence on the thermal relaxation dynamics of the sensor under the action of infrared radiation. Time to achieve sensor stationary output signal is determined by the heat capacity of the membrane C and the heat conductivity of the thermocouple G_t and must be less than the time frame τ_f:

$$\tau \approx \frac{C}{G_t} \leq \tau_f$$

Modeling of the sensor thermal relaxation process allows us to estimate basic parameters – temperature difference between cold and hot contacts of the thermocouples and, consequently, thermopower, volt-watt sensitivity and the minimum resolvable temperature difference (NETD) with taking into account the restrictions which are determined by frame rate, sensor area, physical and geometrical parameters of the layers in its structure.

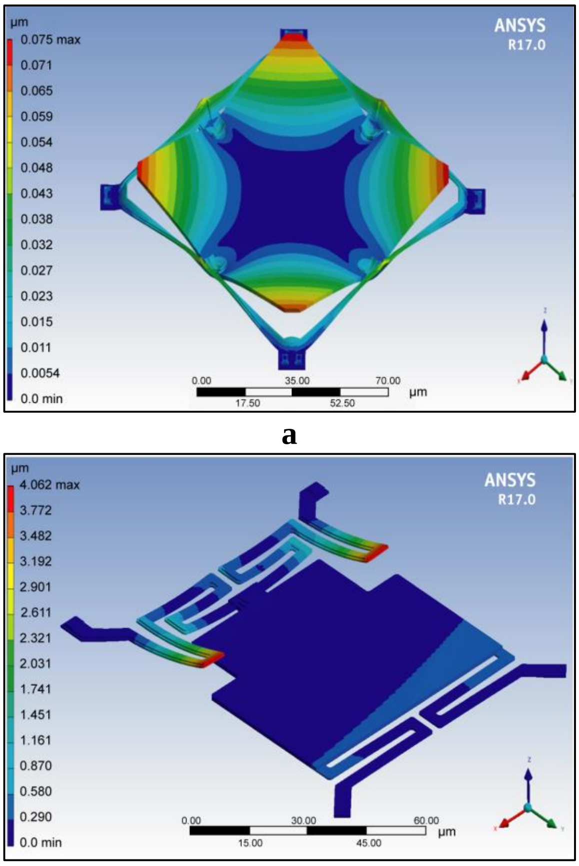
Modeling of nonstationary thermal processes was carried out as follows. The thermally insulated structure of a thermocouple sensor was divided into rectangular zones, depending on the composition and conditions of heat transfer. Each zone was replaced with an equivalent area with homogeneous parameters. For each zone the initial conditions and heat transfer via heat conduction through the edge of the area with neighbouring areas and ground were determined. We did not take into consideration the heat exchange with the environment by heat transfer through the gas medium, i.e. it was considered that the sensor is in a vacuum. It is standard practice for modern thermal sensors matrix.

The conditions of heat exchange with adjacent zones and the substrate via heat conduction through the edges of the zone were set by the boundary conditions on these edges. For each zone the unsteady heat conduction equation was determined and then this equation, boundary and initial conditions for the zone were modified using a direct Fourier transform to eliminate the time variable and go to the frequency field. The transformed equation was solved in the frequency field by the eigenfunction method. The densities of heat flow between the zones which are included into the decision, was presented as sum of orthogonal functions. Then the inverse Fourier transform carried out. Thermocouples thermopower was determined by difference of temperatures between "cold" and "hot" junctions depending on the number of series-connected thermocouples and Seebeck coefficient.

Results and discussion

A. Modeling of deformation

Deformation both in the membrane, and in consoles, which are located on the thermocouple shoulders depend on the combination of materials used to manufacture them. The internal stresses affect both mechanical and optical and electrical properties. The deformation of the membrane plane leads to a change of the membrane absorption coefficient, and tension in the thermocouple shoulders can lead to additional scattering on the deformation potential. This in turn affects the shoulder resistance of the thermocouple and the Seebeck coefficient.



a

b

Fig. 2. The results of the thermomechanical deformations modeling of the membrane and consoles (formation temperature 500C, membrane – SiO_2 absorbing layer is Si_3N_4, thermocouple – Si*, "hot" contact – Al).

Fig. 2 shows typical simulation results of the deformation of the membrane (Fig. 2a) and consoles (Fig. 2b). As can be seen from this figure, the highest stresses occur in areas of broken symmetry: at corner points and points of inflection. Such deformation in practice has been observed for the fabricated test samples.

To study deformations of consoles, the bi-material cantilevers with a length of 100 µm with the width of the lower layer 3 µm and upper layer 2 µm (the thickness of the layers are given in table 1) were selected as the model. For cantilevers were used combinations of materials typical for modern CMOS technologies.

Fig. 3 shows the simulation results of deformations for typical combinations of materials that can be used for the formation of the thermocouple sensor. The figure shows that the greatest deformation arises in the cantilever with the top layer of Al and polysilicon. Moreover, as can be seen from the figure, the deformation as in the case of polysilicon, and the aluminum case has the same sign.

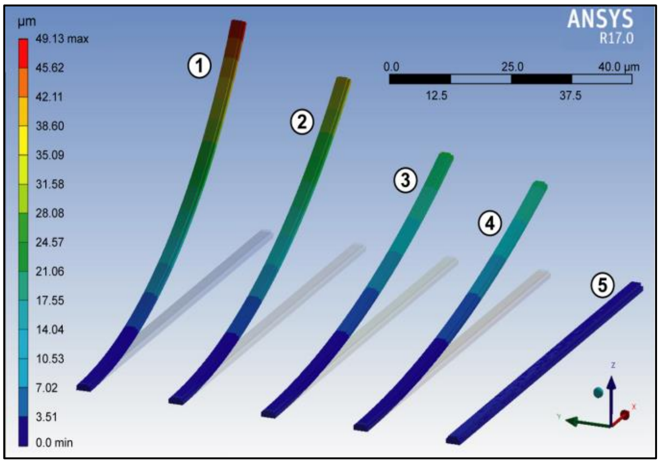


Fig. 3. The results of thermomechanical deformation modeling of bimaterial cantilever (formation temperature 500C): 1 – Al (top)-SiO_2 (bottom), 2 – Al-Si_3N_4, 3 – Si*-SiO_2, 4 – Si*-Si_3N_4, 5 – Si_3N_4- SiO_2

In this case, the cantilever consisting of a film Si_3N_4 - SiO_2, is practically not deformed. This means that the deformation of the membrane shown in Fig. 2a, caused by the presence of aluminum jumpers on the "hot" junctions of the thermocouple. Therefore, it is better to use silicides of refractory metals used in modern CMOS technologies (titanium, tungsten) for the formation of the thermocouple hot junction.

Pair Si_3N_4-SiO_2 was selected as a structure for the membrane, which does not lead to significant deformations. Spectroscopic study of Si_3N_4 films [10] were taken into account which revealed the possibility of achieving high (up to 85%) absorption efficiency of infrared radiation in the range of 8–14 microns. Deformations in consoles with polysilicon thermocouple with high Seebeck coefficient are minimized due to the formation of thermocouple line in the form of a meander, where the console counter lines mutually equilibrate possible normal space deviation. Lateral shifts are not significant so far as the consoles length at the meander vertices are minimal. Longitudinal-axial symmetry of the sensor topology minimizes angular shifts of the membrane. Deformation of the membrane from the Al-contact, which provides the connection of different layers of polysilicon on the «hot» thermocouple junction can be reduced by selecting the minimum allowable size of the contact structure or the application of titanium or tungsten silicides.

As can be seen in Fig. 4, a slight deformation at the level of 1.5-2.3 µm in the sensor structure occur on the thermocouple lines bends. However, the membrane is practically not deformed. The sensor strain with two thermocouples is 1.5 times less because of shorter length thermocouples (Fig. 4b), while the membrane is raised above the substrate approximately 0.5 microns.

Simulation results show the importance of considering the strains in the development of a thermocouple sensor. This is especially true of multi-layered membranes appears when you attempt to increase the absorption coefficient of the heat sensitive.

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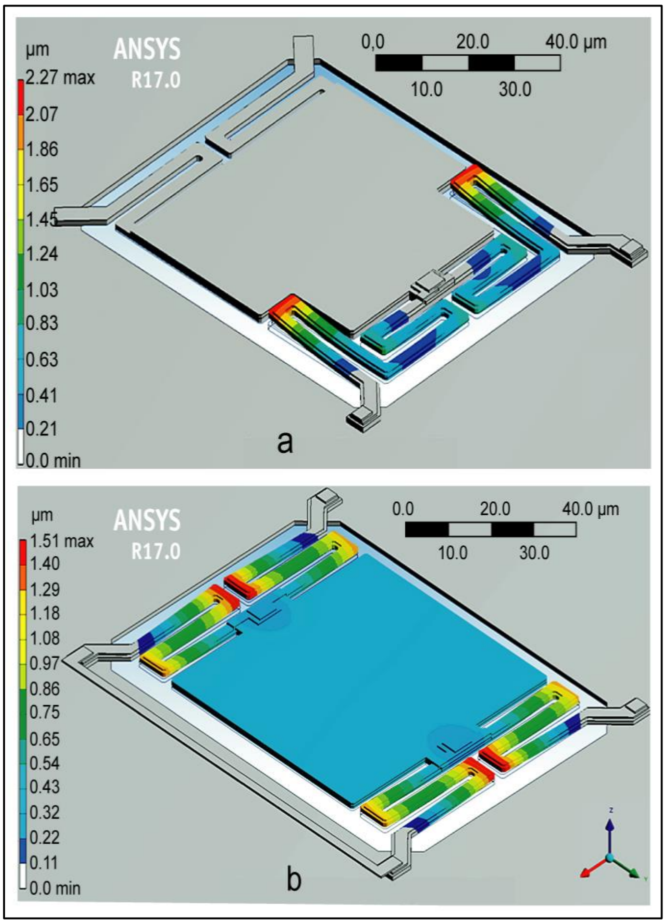

Fig. 4. Modeling of the sensor thermo-mechanical deformations arising in the process of structure formation at 500C:
a) with a single thermocouple, b) with two thermocouples.

B. Simulation of transient process of heat transfer

Fig. 5 presents the results of modeling of membrane temperature relaxation under the action of thermal radiation pulse with intensity of 10^{-3} W/cm^2 and the duration of 0.2 s for the two designs of the sensor.

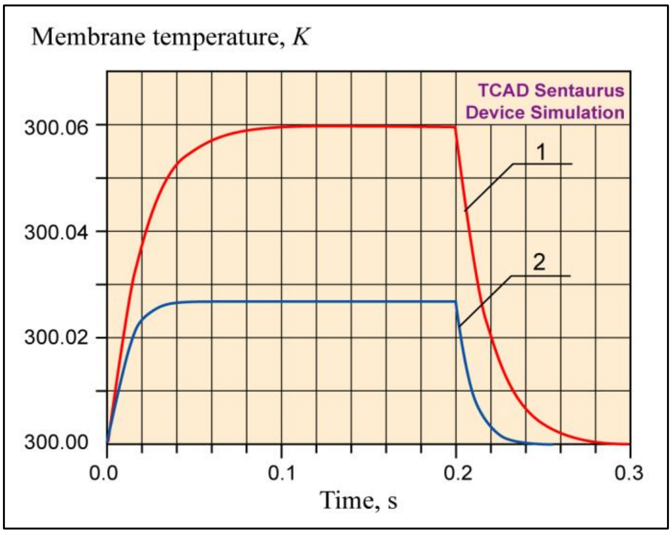

Fig. 5. Thermal relaxation of the sensor membrane by the action of thermal radiation pulse with an intensity of 10^{-3} W/cm^2 and a duration of 0.2 seconds:
1 – sensor with single thermocouple, 2 – sensor with two thermocouples.

Sensor with two thermocouples relaxes faster and shows smaller stationary temperature due to the large heat leaks through the thermocouples. A twofold increase in the thermopower for this design, however, leads to the increase of the total electric resistance of the thermocouple, thereby increasing NETD.

It is necessary to carry out the estimate of the thermocouple sensors parameters, related to their reaction to heat radiation, taking into account the resulting temperature gradients through the area of the membrane.

Fig. 6 shows the temperature map of the thermocouple sensor with single thermocouple under the action of heating by thermal radiation with an intensity of 10^{-3} W/cm^2 at substrate temperature 300K.

It is seen that the temperature of the «hot» junction of the thermocouple is lower than the temperature of the membrane by about 4%. This is quite a lot, because the temperature contrast in the range of 8–14 microns is on the order of one percent. This circumstance is due to the weak thermal conductivity of the sensitive layer of silicon nitride. The use of relatively thin metal underlayer between silicon oxide and silicon nitride eliminates the "cooling" of the membrane in the location of thermal contact thermocouples (metal underlayer is thin reasonably of the correlation between of silicon nitride thermal conductivity and thermal conductivity of the metal, which is of the order of ≈0,1). This underlayer is also available as a reflective coating on the back side of the silicon nitride film, giving an increase in absorption capacity due to repeated passage of radiation.

The results of the simulation of the transient process of the heat transfer enable to estimate the characteristics of the sensor sensitivity.

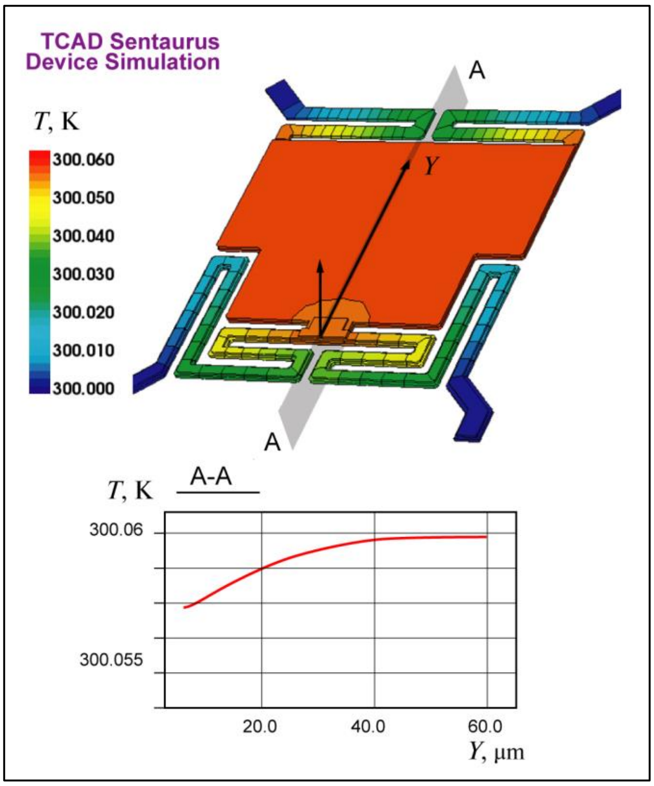

Fig. 6. Temperature distribution through the sensor area under the action of thermal radiation with an intensity of 10^{-3} W/cm^2 at substrate temperature 300K.

The initial data for estimations of the considered constructions of sensors are:

- thermopower $\Delta V = \alpha \Delta T_t$, where α – the Seebeck coefficient of the thermocouple ($\alpha = 300\ \mu V \cdot K^{-1}$), ΔT_t – the created thermocouple temperature difference;
- heat radiation power, absorbed by the membrane $P = A \cdot I$, where A – area of the membrane, I – value of the thermal radiation intensity used in the simulation ($I = 10^{-3} W \cdot \mathrm{sm}^{-2}$);
- temperature change of the object $\Delta T_o = I/\eta q j$, where η – absorption efficiency ($\eta \approx 0{,}9$), q – optics parameter (q <0,25), $j \approx 2{,}62$ W/m^2·K (for 8 – 14 μm);
- thermal noise of the thermocouple $V_n = \sqrt{4 k_B T B R_t}$, where k_B – Boltzmann constant,

T – temperature, B – band width read signal ($B = 2/\tau_f$, τ_f – time frame), R_t – thermocouple electrical resistance ($R_t = R_{sq} l/w$), $R_{sq} = 20$ Ohms per square, w and l – width and the overall length of the thermocouple, respectively.

The simulation results of the considered structures MEMS thermocouple sensors gave the following parameter values.

Sensor with single thermocouple:

- sensitivity $\Delta V/\Delta P \approx 620$ V/W;
- voltage sensitivity to changes in the temperature of the object $\Delta V/\Delta T_O \approx 1{,}0$ μV/K;
- NETD ($\tau_f = 0{,}1$ c) $= V_n \frac{\Delta T_0}{\Delta V} \approx 28{,}7$ mK.

Sensor with two thermocouples:
- sensitivity $\Delta V/\Delta P$ = 455 V/W;
- voltage sensitivity to changes in the temperature of the object $\Delta V/\Delta T_O \approx 0{,}9$ μV/K;
- NETD (τ_f =0,1 c) ≈ 38,4 mK.

Conclusion

Simulation results show the importance of modeling in the development of thermocouple sensors.
First, the simulation allows to identify the picture of the stress distribution in the membrane and consoles and to estimate the absolute magnitude of the deformation. ANSIS simulation allows to obtain quite reasonable results for the distribution of stresses and strains, as confirmed by measurements on test structures. The simulation results of deformations were taken into account for the design of TPA with format 64 x 64.
Second, the simulation of unsteady transient process of heat transfer allowed to reveal function details of the sensor thermocouple, namely: the insufficient heat conduction of the silicon nitride absorbing membrane.
Modeling role is especially important when multilayer absorbing membranes are used. In this case there is the difficult task of taking into account the thermal conductivity between the individual absorbing layers and optimizing of their thicknesses
The results of the transient process simulation of heat transfer in the sensor design allowed us to estimate the sensitivity of the sensor.

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