Modeling the Electromechanical Properties of the MEMS Element of a Thermoelectric Infrared Sensor Based on the Dynamic Seebeck Effect

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Abstract – In this work, we studied the electromechanical properties of the MEMS (micro-electro-mechanical system) element of an infrared (IR) sensor with nanoscale switchable thermocouples for two promising types of its design, depending on the geometry of the electrodes on a square dielectric membrane, controlling its electrostatic displacement – when they are placed on opposite sides of the membrane (design 1) and along its perimeter (design 2), respectively. From the simulation it follows that the threshold voltage corresponding to the contact of the surface of the membrane and the bottom of the cavity in the substrate, as a result of which the heat accumulated in the membrane by IR radiation is dissipated and the microsystem is switched, is almost 5 times lower for the second design of MEMS element than for the first one. It makes the second design more promising not only in terms of energy consumption, but also speed, due to the larger contact area of the membrane with the heat-conducting layer, which reduces the reset time required to return the MEMS element to its original state. The results obtained can be used to create a new generation of matrix photodetector devices operating in the infrared range.

Index Terms – MEMS technology, IR photodetector, nanoscale thermocouples, composite dielectric membranes, electromechanical deformation.

I. INTRODUCTION

In the modern world, the technology of micro-/nanoelectromechanical systems (MEMS / NEMS) becomes especially relevant for creating advanced electronics devices based on miniature sensors (portable gadgets, wireless energy storage devices, virtual reality devices, artificial intelligence (AI) systems, Internet-of-Things (IoT), etc), which are actively used in everyday life. In this context, the development of non-contact detection methods plays an important role for obtaining information about the distribution of temperature fields, which can be applied to the tasks of thermography (in medicine, biology, sports), night vision, monitoring human activity, assisting in unmanned driving, as well as monitoring product quality in industry. It is well known that any object with a non-zero absolute temperature is a source of IR radiation (with a frequency from 0.3 to 400 THz and a corresponding wavelength from 0.75 to 1000 µm), and the intensity and spectral range of such radiation directly depends on the shape, material, and temperature of the object. Thus, the direct detection of the IR spectrum provides a solution to the above problems.

The IR sensors are divided into two groups according to the principle of their operation: 1) thermal IR sensors operating on the electromagnetic (IR) heating of the absorbing layer [3], and semiconductor photon (quantum) IR sensors, the principle of detection of which is based on the generation of electrons and holes by incident IR radiation [4]. Despite the fact that photon IR sensors have a good signal to noise ratio and a fast response, however, they operate in a relatively narrow spectral range and require an expensive cooling system, while their noise characteristics deteriorate with temperature. Unlike IR detectors based on photon-absorbing semiconductor materials, thermal IR sensors with sensing thermocouples are energy efficient, provide a linear spectral response in a wide range of wavelengths, practically do not have flicker (1/f) noise and can operate without cooling, which opens the way to creating inexpensive portable and low-power thermal imaging systems [5-7].

II. PROBLEM STATEMENT

However, towards the optimization of existing prototypes of such devices, there is a dilemma associated with the impossibility of simultaneously achieving good thermal insulation of the IR-absorbing layer (to increase the sensitivity of the sensor) and an acceptable heat sink sufficient to prevent dramatic heating of the MEMS element by incident IR radiation, which can lead to the degradation of sensitive thermocouples. Thus, the urgent task is to search for new design solutions that will help to withstand high temperatures and provide good thermal insulation of the sensitive element, which is necessary to eliminate the residual thermal image after reading and becomes crucial for the stable operation of the IR sensor, especially in the case of small pixel sizes of the thermal imaging matrix [8, 9].
III. THEORETICAL MODEL OF MEMS ELEMENT WITH THERMOCOUPLES

The research problem analyzed in this paper relates to the task of developing a new type of uncooled microsystem with switchable thermocouples for thermolectric IR sensor, which is based on the non-stationary Seebeck effect [10]. The scientific novelty of the proposed solution is associated with the original dynamic principle of the MEMS thermocouple, which will provide a significant improvement in the signal-to-noise ratio and simplify the signal processing in infrared image receivers used in thermal imaging. The originality of the considered designs of the MEMS element as a part of the thermolectric IR sensor is based on the solutions proposed earlier by our group in [11, 12] and which ensure the high efficiency of the MEMS-based IR sensor, which can be confirmed by numerical simulation of the electromechanical deformation of film microstructures. In turn, the choice of the topology of the switchable thermocouple for the thermolectric IR sensor can be determined by a number of factors, namely: the limitation of the area of the MEMS element, technological limitations associated with the minimum dimensions of the topological fragments of the structure, physical and structural parameters of the materials used to form the structure of the sensitive element, and, finally, the required performance characteristics of IR detector. An important circumstance that must be taken into account during design is that the sensitivity of the MEMS element to thermal radiation is provided by a membrane, which must be isolated from the substrate. This is realized by means of flexible consoles that hold the membrane in a suspended state and act as supporting elements for the thermocouples located on them. The design of the consoles should ensure minimal heat leakage and, if possible, compensate for deformations arising from the heat treatments required to form the topological pattern of the MEMS element.

A. Design and principle of operation

The MEMS element of the thermoelectric IR sensor considered in this work consists of the following components - a perforated square-shaped membrane fixed on movable consoles, a system of gate electrodes (to which a control voltage is applied) and a system of sensitive thermocouples (Fig. 1). Taking into account the capabilities of the technological equipment used to form MEMS structures, the topology of the MEMS element was designed for the 0.8 μm technology node.

A thin (450 nm) layer of Si3N4 was chosen as the material of the membrane and consoles. In order to improve the thermal absorption performance of MEMS-element, a layer of non-stoichiometric silicon nitride (SiNX) with a thickness of 600 nm is deposited on the membrane, which ensures the sensitivity of the element to thermal (IR) radiation in the wavelength range of 2.0–16.0 μm. The membrane has a sensitive area of 100x100 μm2. The heat from IR radiation is absorbed by the membrane, this microcavity provides heat rejection when the membrane surface comes into contact with the cold part of the thermocouple on the substrate. The microcavity is located under the membrane, which is formed as a result of etching of the sacrificial layer with an area equal the size of the sensitive region (100x100 μm2). In addition to thermal insulation of the membrane, this microcavity provides heat rejection when the membrane surface comes into contact with the bottom, which is achieved in the process of its electromechanical deformation at a given threshold voltage applied to the n+- doped Si* gate electrodes. Fig. 2a shows two sketches of the topology of the MEMS element with sensitive thermocouples, which differ in the geometry of the gate electrodes. In the first type of design, the ends of the electrodes are located on two opposite sides of the square membrane, while in the second one the gate electrode is placed along the entire perimeter of the membrane. Based on the corresponding topologies of the MEMS element, two three-dimensional models of its design were developed in
the Comsol MultiPhysics software [13], which is illustrated in Fig. 2b-c. These models were made to analyze the electrostatic deformation of the perforated membrane in the designs proposed. This will allow us to calculate the threshold voltage of heat discharge after the read operation, evaluate the corresponding performance and optimize the design of the MEMS element of the thermoelectric IR sensor. As an option, it is also possible in our models to add grooves to the bottom of the microcavity in places located opposite the flexible membrane consoles.

Fig. 2. Sketches of the topology of the MEMS element of the thermoelectric IR sensor (without wiring) and the corresponding three-dimensional models (from Comsol MultiPhysics) of its design, with the electrodes located (a) on two opposite sides and (b) around the perimeter of a perforated square membrane.

From a technological point of view, such a modification is considered as one of the ways to prevent the consoles from contacting the cavity bottom during electrostatic deformation, which can lead to irreversible destruction of the whole microsystem.

B. Basic equations

In order to calculate the deformation of a thin-film dielectric membrane \( \text{Si}_3\text{N}_4 \) (130 nm) / \( \text{Si} \) (600 nm) / \( \text{Si}_3\text{N}_4 \) (130 nm) under the action of an electric field generated between the gate electrodes and the substrate, the «Electromechanics» module was used as a part of the Comsol MultiPhysics software package [13]. This module is based on the solution of the Euler-Cauchy differential equation, which describes the deformation \( \mathbf{u} \) of linear elastic materials under the influence of an external electromechanical load:

\[
\rho \frac{d^2 \mathbf{u}}{dt^2} = \nabla \cdot \sigma_{\text{EMV}} + \mathbf{f}_e,
\]

where \( \rho \) is the density of the material, \( \mathbf{u} \) is the structural displacement vector, \( \sigma_{\text{EMV}} \) is the electromechanical stress tensor (Maxwell stress tensor), \( \mathbf{f}_e \) is the external force acting on the material (e.g. gravity). In stationary mode, when there is no acceleration, \( \nabla \cdot \sigma_{\text{EMV}} + \mathbf{f}_e = 0 \). Also, the stress tensor must be continuous at the boundary between materials, which corresponds to the fulfillment of the next boundary conditions:

\[
\mathbf{n}_j \left( \sigma_{\text{EMV}(i+1)} - \sigma_{\text{EMV}(i)} \right) = 0,
\]

where \( \sigma_{\text{EMV}(i)} \) (\( \sigma_{\text{EMV}(i+1)} \)) is the stress tensor in the \( i \) (\( i+1 \)) - th material, \( \mathbf{n}_j \) is the normal vector to the boundary of the \( i \) - th material.

The electromechanical stress tensor in a vacuum space (in the absence of magnetic fields) is described by the equation:

\[
\sigma_{\text{EMV}}^{(\text{vac})} = \varepsilon_0 \mathbf{E} \otimes \mathbf{E} - \frac{1}{2} (\varepsilon_0 \mathbf{E} \cdot \mathbf{E}) I,
\]

where \( \mathbf{E} \) is the vector of the electric field in the microcavity (between the substrate and the membrane), \( I \) is
the identity tensor, $\varepsilon_0$ is the permittivity of free space, and $\left(\mathbf{E} \otimes \mathbf{E}\right)_{ij} = E_i E_j$. The field $\mathbf{E} = -\nabla V$ is calculated from the solution of the Poisson equation for the potential distribution $\nabla^2 V = -\rho_v / \varepsilon_0$, where $\rho_v$ is the charge density. For small strains, the electromechanical stress tensor in an isotropic linear dielectric that does not have electrostrictive properties is determined by a relationship of the form:

$$\sigma_{\text{EMV}}^{\text{dielec}} = \varepsilon_0 \varepsilon, \mathbf{E} \otimes \mathbf{E} - \frac{1}{2} \varepsilon_0 \varepsilon, \left(\mathbf{E} \cdot \mathbf{E}\right) I = \sigma_{\text{EMV}}^{\text{vac}} + \varepsilon_0 \chi_0 \left[\mathbf{E} \otimes \mathbf{E} - \frac{1}{2} \left(\mathbf{E} \cdot \mathbf{E}\right) I\right] \tag{4}$$

where $\chi_0$ is the dielectric susceptibility of the material.

Following the equations (1) - (4), the balance of forces at the boundary between the dielectric membrane and vacuum (or air) can be described as:

$$\mathbf{n}_{\text{dielec}} \left[\left(\sigma_{\text{EMV}}^{\text{dielec}} + \rho_{\text{air}}\right) - \left(\sigma_{\text{EMV}}^{\text{dielec}} + \sigma_m\right)\right] = 0 \tag{5}$$

where $\sigma_m$ is the mechanical component of the total stress, $\rho_{\text{air}}$ is the air pressure (if present), $\mathbf{n}_{\text{dielec}}$ is the normal vector to the surface of the dielectric membrane. At the same time, it should be taken into account that the boundary condition described by equation (1) is satisfied at the interfaces of the layers of the $\text{Si}_3\text{N}_4 / \text{SiN}_x / \text{Si}_3\text{N}_4$ dielectric membrane. Since the gravity force slightly affects the final results of numerical calculations, it was not taken into account during the simulation.

IV. SIMULATION RESULTS

The results of modeling the electrostatic displacement of the membrane as part of the considered microsystem designs are presented in Fig. 3. A voltage in the range from 0 to 30 V was applied to the gate electrodes, while the typical deformation of the membrane is given in Fig. 3 for the case when the voltage $V_A = 15$ V is applied to the gate electrodes. Figure 3a illustrates the electrostatic deformation of the first design of the MEMS element (with gate electrodes located opposite to each other), and the maximum displacement is observed for flexible meander consoles on which gate electrodes are placed, which is most likely due to their asymmetric geometric configuration. In turn, the membrane moves towards the bottom of the cavity practically without any distortion in the XOY plane (i.e. parallel to the bottom plane).

In the second type of design of the MEMS element, where the electrode passes along the entire perimeter of the membrane, only one side of the membrane is electrostatically displaced, while the opposite part remains almost motionless (Fig. 3b). This feature is due to the fact that this side of the membrane lies on a flexible console that repeats the shape of two thermocouples fixed on two contact pads near the edge of the cavity, which enhances the mechanical strength of the structure in this area and makes the electrostatic deflection of the membrane asymmetric. Fig. 4 shows the comparative dependences of the membrane deformation on the applied voltage for the two designs of the MEMS element considered, from which the value of the threshold voltage corresponding to the moment when the membrane touches the bottom of the cavity is calculated. Since the microcavity depth is only 0.8 μm, the membrane contacts the cavity bottom at relatively low voltages - 29.3 V for the first type, and 5.9 V for the second type of design of the MEMS element, respectively. The membrane deformation is seen to monotonically increase with increasing applied voltage.
Substrate by means of flexible consoles (with an intermediate non-stoichiometric SiNx layer that absorbs IR radiation), the system of (n+) - doped Si* gate electrodes, and the system of (n+/p+) Si* sensitive thermocouples. Thermocouples and gate electrodes are considered for two types of the MEMS element design: 1) when the electrodes are placed on two opposite sides of the square membrane and 2) when the electrodes are located around the perimeter of the membrane (ring geometry). The possibility of adding grooves to the bottom of the cavity in the substrate in places located opposite the elastic consoles was also considered, in order to prevent their contact with the bottom of the cavity during electrostatic deformation. Based on the developed models, the dependences of the membrane deformation on the control voltage in the range from 0 to 30 V were obtained for two versions of the microsystem design. It is shown that for the same voltage applied to the gate electrodes the membrane deformation in the case of the ring geometry of the gate electrode (design 2) will significantly exceed the deformation obtained in another case (design 1). Thus, the topology of the MEMS element with ring geometry of gate electrode is more effective, since it allows reducing several times the threshold voltage of the electrostatic microsystem switching. The results obtained in this work can be used during the development and optimization of a matrix receiver of IR radiation based on MEMS elements with sensitive thermocouples [12, 14].

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