Fully quantitative characterization of CMOS–MEMS polysilicon/titanium thermopile infrared sensors

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This study demonstrates a fully quantitative characterization of a highly sensitive CMOS–MEMS polysilicon/titanium thermopile infrared sensor by using the simulations of non-sequential ray tracing and solid conduction, and the measurements of voltage response and frequency response in atmosphere and in vacuum.

The thermal time constants of 17.0 ms in air and 37.0 ms in vacuum for the polysilicon/titanium thermopile with a gold-black absorber were estimated by the measurements of frequency response. The solid conductance, gas conductance, radiation loss, and heat capacitance of the thermopile were characterized as 112 μW/K, 141 μW/K, 5.88 μW/K, and 4.40 μJ/K in atmosphere by the simulation of solid conduction using ANSYS and the measurements of frequency response. The voltage responsivity, sensor noise, noise equivalent power, and specific detectivity of the gold-black coated thermopile in air were estimated as 63.1 V/W, 27.0 nV/Hz^1/2, 0.43 nW/Hz^1/2, and 1.87 × 10^8 cm Hz^1/2/W by the simulation of received optical power using LightTools ray tracing software and the measurements of voltage response. It shows that the sensor has the highest specific detectivity compared to the published CMOS–MEMS thermopiles in atmosphere due to the design of low solid conductance and high emissivity. Eventually, the Seebeck coefficient of the polysilicon/titanium pair was first evaluated and has a magnitude of 170.2 μV/K.

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1. Introduction

Thermopile infrared sensors were widely used as the sensing elements of nondispersive infrared (NDIR) gas detectors [1,2], thermal imagers [3,4] and non-contact infrared thermometers [5]. Thermal imagers and infrared thermometers are the devices that transform infrared radiation into temperature reading. NDIR gas detectors consist of band-pass filters, infrared emitters, and infrared sensors which could detect the concentration of specific gases by the signal difference resulted from the absorption of infrared power by the gases. In order to enhance the selectivity of gas sensing, the bandwidths of the band-pass filters are usually preferred to be as narrow as the absorption bandwidths of the specific gases which would result in the weak and slight received infrared power of the sensors. It is particularly important and necessary to develop a highly sensitive infrared sensor for NDIR gas sensing. Thermopiles are thermal-type infrared sensors which transfer thermal radiation into thermoelectric voltage. Therefore, the performances of thermopiles, such as responsivity, specific detectivity and response speed, are quite dependent on their thermal properties. A thermopile sensor comprises many thermocouples connected in series and the connections of the thermocouples divide into hot junctions and cold junctions. In general, the hot junctions are thermally isolated from their substrate and an infrared absorber is coated onto the surface of the thermopile for improving the sensitivity of the infrared sensor. As a thermopile absorbs the infrared radiation emitted from an infrared source, the temperature difference between hot junctions and cold junctions is formed and the thermoelectric voltage between the two terminals of thermocouples in series is created at the same time. The magnitude of the output voltage is directly proportional to the number of thermocouples, the Seebeck coefficient of the thermocouple material pair, and the temperature difference between hot junctions and cold junctions. And the temperature difference is in direct ratio to the emissivity of the infrared absorber, received infrared power, and the reciprocal of thermal conductance. The voltage responsivity of an infrared sensor is defined as the ratio of output voltage to received infrared power which specifies the input–output gain of a sensor system. However, specific detectivity is the most important specification of an infrared sensor to indicate the signal-to-noise.

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ratio of an optical sensor. The magnitude of specific detectivity for a thermopile infrared sensor is in direct proportion to the emissivity of the infrared absorber, the Seebeck coefficient, and the reciprocal of thermal conductance. The main heat losses for thermopile devices are solid conduction and gas conduction since the radiation loss is relatively small and negligible. For thermal microsensors, the gas conductance may even dominate the behavior of heat transfer and the performance in atmosphere [6,7]. In addition, the response time constants of thermal devices, which are defined as the ratio of heat capacitance to thermal conductance, are also highly dependent on their thermal properties. It shows that the quantitative characterization of the thermal properties is very useful and valuable for the analysis of the sensor performances and the design of thermal sensors.

For the reasons of mass production, IC integration, and low cost, a CMOS compatible process was frequently employed as the front-end process of a MEMS thermopile infrared sensor [8–11,3,4,12–15]. In past years, polysilicon and aluminum were the most common materials for forming the thermocouple pairs of CMOS thermopiles since the fabrication process of a polysilicon/metal (poly/al) thermopile is relatively simple and compatible. However, the thermal conductivity of a CMOS aluminum film is about 200 W/mK [16] which is an order of magnitude greater than those of polysilicon and titanium [17]. The high solid conductance of a polysilicon/aluminum (poly/al) thermopile could result in a low sensitivity. Besides, an interference structure was used to serve as an infrared absorber of a CMOS–MEMS thermopile which has low absorptance and a narrow absorption bandwidth [2,18]. Instead, a porous gold black film with absorptance of >90% and wide absorption band was proposed for thermal infrared detectors [19–21]. In our work, the purpose of the design of polysilicon/titanium (poly/Ti) thermopiles is to improve the specific detectivity of sensors by highly reducing the solid conductance and increasing the emissivity of the infrared sensor without much lowering the Seebeck coefficient and raising Johnson noise. Furthermore, the post process of the thermopile was designed to be a simple photomaskless process. In order to extremely lower the solid conductance of a poly/metal thermopile, a 0.6-μm aluminum film in the standard first metallization process was replaced by a 0.1-μm titanium film with a low thermal conductivity. The Seebeck coefficients of a poly/Ti pair and a poly/al pair should be almost the same since polysilicon has much larger absolute Seebeck coefficient than those of titanium and aluminum [18,22–24]. Besides, the Johnson noise of a poly/Ti thermopile is almost equivalent to that of a poly/al thermopile with an identical layout since polysilicon dominates the electric resistance of the sensor. After the CMOS process, the suspended structure of the poly/Ti thermopile was formed by front-side anisotropic etching of silicon in a dual-doped TMAH solution with low etch rate of exposed aluminum pads [25]. For further lessening solid conductance, accelerating etching process and achieving a high fill factor, narrow and long line-shaped etching windows were designed and located between the thermocouples. Eventually, a porous gold black layer was thermally evaporated onto the surface of the sensor and patterned in situ by metal mask technique to achieve high absorption of infrared power. This paper is focused on the characterization of all the important thermal properties and performances of the poly/Ti thermopile, such as the solid conductance, gas conductance, radiation loss, heat capacitance, thermal time constant, emissivity, Seebeck coefficient, responsivity, Johnson noise, shot noise, temperature fluctuation noise, noise equivalent power (NEP), and specific detectivity, by adopting the LightTools ray tracing simulation of received infrared power, the ANSYS finite element analysis (FEA) of solid thermal conduction, and the measurements of voltage response, frequency response and vacuum response.

2. Theory, design and simulation

2.1. Theory

The thermal behavior of a packaged thermopile under an infrared radiation of \( \Phi \) is governed by the heat flow equation [26]

\[
\frac{dT_h}{dt} + G(T_h - T_c) = \varepsilon \Phi,
\]

where \( T_h \) is the heat capacitance of the thermopile sensor, \( T_c \) is the temperature of hot junctions, \( t \) is the time, \( G \) is the thermal conductance between hot junction and its surrounding with a temperature of \( T_c \) and \( \varepsilon \) is the emissivity which reveals the absorptance of the infrared absorber. The solution of the temperature difference \( \Delta T \) between the hot junctions and its environment in the transient state is [26]

\[
\Delta T = \frac{\varepsilon \Phi}{G} \frac{1}{\sqrt{1 + \alpha^2 T^2}},
\]

where \( \omega \) is the modulated angular frequency of the incident infrared power, and \( \tau = C/G \) is the thermal time constant of the sensor.

The output thermoelectric voltage \( V \) caused by the rising temperature of hot junctions can be expressed by

\[
V = N \alpha_{AB} (T_h - T_c),
\]

in which \( N \) is the number of thermocouples in series, \( \alpha_{AB} \) is the Seebeck coefficient between the two thermocouple materials, \( T_c \) is the temperature of cold junctions which is almost the same magnitude with the ambient temperature \( T_{amb} \). Therefore, the voltage responsivity \( R_v \) of the thermopile can be given by

\[
R_v = \frac{V}{\Phi} = \frac{N \alpha_{AB} \varepsilon}{G} \frac{1}{\sqrt{1 + \alpha^2 T^2}} = \frac{R_{v0}}{\sqrt{1 + \alpha^2 T^2}},
\]

where \( R_{v0} = N \alpha_{AB} \varepsilon/G \) is the flat-band responsivity in the thermal steady state. For CMOS poly/metal thermopiles with the same layout, the number of thermocouples is fixed and the variances of the Seebeck coefficients between polysilicon and CMOS–metals are very small since polysilicon dominates the thermoelectric effect of the poly/metal thermopiles. Therefore, the responsivity of the poly/metal thermopiles in the thermal steady state is almost only in direct ratio to their emissivity and the reciprocal of thermal conductance.

As shown in Fig. 1, there are three types of heat losses that arise in a MEMS thermopile: solid conduction, gas conduction and radiation. As the suspended structure of a thermopile absorbs the incident infrared power radiated from a target, some heat dissipates through the solid suspended structure to silicon substrate.

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**Fig. 1.** Heat transfer of a MEMS thermopile.
The solid conductance \( G_s \) is directly proportional to the thermal conductivity \( k_s \) of the suspended structure and is expressed by

\[
G_s = \frac{k_s \cdot w d}{l},
\]

where \( w, d \), and \( l \) are the width, thickness, and length of the supporting leads of the suspended membrane. And some heat is transported to the substrate by the collisions of gas molecules between the hot suspended membrane and the substrate within the cavity. The gas conductance \( G_g \) is in direct ratio to the free molecular conductivity of gas \( k_g \), and the area of the infrared sensor \( A_s \). Besides, the gas conductance is a function of pressure \( P \) [7,27]. For a thermopile with one-side heat sink, the gas conductance is given by

\[
G_g = \frac{\phi}{2 - \phi} k_b A_s P \left( \frac{P_1}{P_1 + P_2} \right),
\]

where \( \phi \) is the accommodation coefficient of gas, \( P_i \) is an empirical transition parameter which is directly proportional to the reciprocal of gap depth between the device and heat sink [27]. As the pressure \( P_1 \) is negligible compared to the transition pressure, the gas conductance is directly proportional to the pressure of the cavity. It means that a vacuum package is very useful to diminish the gas conductance. Radiation loss is the phenomenon of heat exchange through a thermal device and its environment. The radiation conductance \( G_r \) could be derived from the Stefan–Boltzmann law and given by

\[
G_r = \varepsilon + \varepsilon_b \alpha A_s \left( T_h^2 + T_a^2 \right) \approx 4 \varepsilon + \varepsilon_b \alpha A_s T_a^3,
\]

where \( \varepsilon_b \) is the emissivity of the bottom surface of the sensor, \( \alpha \) is the Stefan–Boltzmann constant, and the temperature of hot junctions is considered to be close to the ambient temperature since the temperature rising of hot junctions under thermal radiation is tiny. The total thermal conductance of a thermopile sensor is given by

\[
G = G_s + G_g + G_r.
\]

In general, the radiation conductance of a thermopile is negligible since the temperature of hot junctions is only slightly higher than the ambient temperature. However, the gas conductance of a MEMS thermal device in atmosphere is significant due to the miniature dimension of cavity gap. For reducing the gas conductance, a vacuum or a filling-gas environment was often used by published papers and manufacturers [18].

The main noise source of a thermopile sensor is Johnson noise due to no bias supply requirement during the sensor’s operation [28]. Johnson noise is expressed as

\[
\eta_j = \sqrt{4k_b T_s R_s \Delta f},
\]

where \( k_b \) is the Boltzmann constant, \( T_s \) is the absolute temperature of the thermopile, \( R_s \) is the resistance of the sensor, and \( \Delta f \) is the noise bandwidth. In addition, shot noise is given by [26]

\[
\eta_s = R_s \cdot \sqrt{2qI_0 \Delta f},
\]

in which \( q \) is the elementary charge of an electron, and \( I \) is the current. The temperature fluctuation noise resulted from the temperature fluctuation \( \left( \Delta T^2 \right)^{1/2} \) in background is written by [26]

\[
\eta_{TF} = N_{\alpha \beta \epsilon} \cdot \left( \frac{\Delta T^2}{2} \right)^{1/2} = \frac{R_0}{\epsilon} \sqrt{4k_b T_s G \Delta f},
\]

where \( \Delta f = \frac{1}{4\pi} \) is the bandwidth of temperature fluctuation noise. The total sensor noise of a thermopile sensor is expressed as

\[
\eta_t = \sqrt{\eta_j^2 + \eta_s^2 + \eta_{TF}^2}.
\]

Noise equivalent power \( NEP \) and specific detectivity \( D^* \) are the most significant specifications of an infrared sensor to qualify the signal-to-noise performance of the sensor. \( NEP \) is defined as the received infrared power which has a signal-to-noise ratio of 1. The \( NEP \) of a thermopile in the steady state can be expressed and approached as

\[
NEP = \frac{\varepsilon_a}{R_V} = \frac{G}{N_{\alpha \beta \epsilon}} \sqrt{4k_b T_s R_s \Delta f}.
\]

For a poly/metal thermopile, the polysilicon lines dominate the resistance and the thermoelectric effect of the sensor. Consider a simple polysilicon cantilever which has a dimension of \( L \) in length, \( w_p \) in width, \( d_p \) in thickness, and a resistivity of \( \rho_p \), the resistance \( r \) of the cantilever along the length of polysilicon line is given by

\[
r = \rho_p \frac{L}{w_p d_p}.
\]

If the polysilicon cantilever is divided into \( N \) equal lines with the same width of \( w_p / N \) by considering that the intervals between the polysilicon lines are negligible. Then the resistance of the polysilicon lines in series could be written as

\[
r_s = N \cdot \rho_p \frac{L}{w_p / N d_p} = N^2 r.
\]

And the \( NEP \) can be rewritten as

\[
NEP = \frac{G}{N_{\alpha \beta \epsilon}} \sqrt{4k_b T_s r \Delta f}.
\]

It shows that the dependence of \( NEP \) on the thermocouple number \( N \) disappears due to the rapidly increasing of sensor resistance. \( D^* \) is defined as the reciprocal of \( NEP \) and normalized to the sensor area \( A_s \) and the bandwidth \( \Delta f \)

\[
D^* = \frac{\sqrt{A_s \Delta f}}{NEP} = \frac{\alpha_{\alpha \beta \epsilon}}{G} \sqrt{A_s} \frac{1}{4k_b T_s r}.
\]

It implies that the magnitude of \( D^* \) is almost only dependent on the emissivity and the thermal conductance of the sensor for a poly/metal thermopile with the same process and sensor size.

In this work, the absorption spectrum of the absorber layer was measured by using Fourier transform infrared spectrometry (FTIR) in order to estimate the emissivity \( \epsilon \) of the poly/Ti thermopile infrared sensor [5]. According to the statement of Kirchhoff’s law of thermal radiation, the emissivity of a body equals its absorptivity at thermal equilibrium. Therefore, the emissivity of the absorber layer could be evaluated by the calculation of average absorptivity of infrared radiation over a specified wavelength range.

The important performances of thermopiles were evaluated by the simulation of received optical power, the measurement of thermoelectric voltage, and the theoretical calculation of sensor’s noises. In order to estimate the received power \( \Phi \) of a TOS–packaged thermopile at various temperatures of a blackbody infrared source and at ambient temperature, a ray tracing simulation was carried out by adopting LightTools software. The responsivity of the thermopile is defined as the ratio of the output thermoelectric voltage \( V \) to the received optical power \( \Phi \), in which the output voltage was obtained by the measurement of sensor’s voltage response under infrared radiation and the corresponding received optical power was simulated by LightTools. The sensor noise \( \eta_t \) of the thermopile is calculated by using Eqs. (9)–(12) and the \( NEP \) of the sensor was evaluated by calculating the ratio of sensor noise to responsivity. Subsequently, the specific detectivity \( D^* \) could be further given by utilizing its definition in Eq. (16).

The thermal properties of thermopiles were further found and analyzed by the simulation of solid conductance, the measurements of frequency responses in air and in vacuum. To estimate the solid conductance of thermopile sensors, the temperature distributions of hot junctions under infrared radiation was simulated by adopting ANSYS FEA software. In the simulation, an exact 3D model of a poly/metal thermopile chip was constructed and the
4. Conclusion

A CMOS–MEMS gold-black coated poly/Ti thermopile infrared sensor with a high specific detectivity was fabricated by using a 0.8−μm six-mask CMOS process and a post process without any lithography step. The thermal properties and performances of the poly/Ti sensor have been fully characterized by simulations and measurements in this study. The characterization results show that the poly/Ti thermopile has excellent responsivity and specific detectivity of 63.1 V/W and 1.87 × 10^8 cm Hz^{1/2}/W due to the low thermal conductivity of titanium. The specific detectivity of the CMOS poly/Ti thermopile with the designs of low thermal conductance and high emissivity is 6.1 times higher than that of standard CMOS poly/AI thermopiles without gold black coating. The contributions of solid conduction, gas conduction and radiation loss on the heat losses of the thermopile were about 43%, 55% and 2%. And the gas conductance could be further neglected and the specific detectivity of the sensor would be raised to 4.06 × 10^8 cm Hz^{1/2}/W by operating under a pressure less than 0.02 Torr. Moreover, the Seebeck coefficient of n+-polysilicon and titanium was first estimated and has a magnitude of 170.2 μV/K. It shows that polysilicon material dominates the Seebeck coefficient of CMOS–MEMS poly/metal thermopiles.

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References


Biography

Chung-Nan Chen was born in Taiwan. He received the B.S. degree in physics from Chinese Culture University, Taipei, Taiwan, in 1988. He received the Ph.D. degree in electro-optical engineering from National Chiao Tung University, Hsinchu, Taiwan, in 1993 and 2000, respectively. His Ph.D. dissertation is the technology development of microbolometer IRFPA detectors. He served for two years in the Taiwan Army. He was with Opto Tech Corporation, Hsinchu, Taiwan; he was involved in the R&D of MEMS products and became a deputy manager of the Division of Microelectronics from 1996 to 2005. In 2005, he became an Assistant Professor with the Institute of Photonics and Communications, National Kaohsiung University of Applied Sciences, Kaohsiung, Taiwan. His research interests include thermal sensors, MEMS and semiconductor process, and infrared engineering.