Comparison of Mechanical Deflection and Maximum Stress of 3C SiC- and Si-Based Pressure Sensor Diaphragms for Extreme Environment

^aNoraini Marsi, ^aBurhanuddin Yeop Majlis, *SMIEEE*, ^aAzrul Azlan Hamzah and ^bFaisal Mohd-Yasin, *SMIEEE*

^aInstitute of Microengineering and Nanoelectronics (IMEN)
Universiti Kebangsaan Malaysia (UKM)
43600 UKM Bangi, Selangor, Malaysia

^bQueensland Micro- and Nanotechnology Centre (QMNC)
Griffith University, 4111, Brisbane, QLD, Australia
Email: burhan@vlsi.eng.ukm.my

Abstract-The design of a capacitive-sensing pressure sensor for extreme environment is proposed in this project. The movable diaphragm (top plate) is made of either cubic silicon carbide (3C-SiC) or Silicon (Si), while the fix diaphragm (bottom plate) is made of Si. This paper specifically compares the mechanical performance of the movable diaphragm utilizing both materials. Two important parameters associated with the behavior of the diaphragm are examined, namely the maximum deflection and maximum stress, and they are simulated at a pressure of 0-100 MPa, and at temperature of 27-1000 °C. The graphs of maximum deflection and stress vs pressures at different temperatures and thicknesses are plotted to summarize the data. SiC diaphragm has lower deflection and stress compares to Si diaphragm at different thicknesses, pressures and temperatures. Then, a linear regression analysis is performed to determine the R-square value. It is shown from these analyses that SiC diaphragm exhibits better linear behavior compares to Si diaphragm. Generally, this work proves that SiC is a better material over Si for the development of a pressure sensor at extreme environment.

Keywords: silicon carbide (SiC), pressure sensor, harsh environment, diaphragm

I. INTRODUCTION

The operating temperature inside the gas turbine engine is typically greater than 300°C [1]. However, the silicon-based MEMS pressure sensor could only operate below this point due to the limitation of its material properties. In such extreme environment, SiC is the best material to replace Si because it can operates up to 1000°C [2]. In addition, SiC has more advantages at this environment due to its chemical inertness and corrosion resistance, and an extremely low coefficient of thermal expansion and high Young's Modulus. The latter is a good mechanical advantage because that makes SiC more immune to stress effects from deflection and thermal shock. Electrically speaking, SiC has an excellent properties compares to Si as well, namely a larger bandgap (2.3-3.4eV), a higher breakdown field (30x10⁵ V/cm), a higher thermal conductivity (3.2 - 4.9 W/cm K), and a higher saturation velocity (2 x 10⁷cm/s) [3]. This paper will demonstrate the superiority of SiC material over Si as the pressure sensor diaphragm through a series of simulations.

II. THEORY AND DESIGN

A. Design of a capacitive pressure sensor

A structural model for the pressure sensor is shown in Figure 1. It consists of two components to make the parallel-plate structure; the first is the top diaphragm as the movable plate, and the second is a bottom substrate as a fixed plate. The pressure signal comes from the top and generates the stress-deformation of the movable diaphragm, which modulates the sealed air gap length. The corresponding differential capacitance value between the top and bottom plates is measured as the electrical output. In this design, the square shape diaphragm with the area of 400 μm² is employed. The thickness of the top movable diaphragm is simulated at the following points: 0.05μm, 0.1μm, 0.2μm, 0.3 μm, 0.5μm and 1.0μm to study the stress deformation of both SiC and Si membranes at different thicknesses.

TABLE I MATERIAL PROPERTIES OF TESTED MATERIALS [4]

Material properties	Silicon	SiC
Young's modulus (GPa)	1.69	4.70
Poisson ratio	0.30	0.22
Density (kg/μm ³)	2.5 x 10 ⁻¹⁵	3.2 x 10 ⁻¹⁵
TCE Integral Form (1/K)	2.50 x 10 ⁻⁶	2.30 x 10 ⁻⁶
Thermal Conductivity (pW/umK)	1.48 x 10 ⁻⁸	5.0 x 10 ⁻⁸
Specific Heat (PJ/kgK)	7.12 x 10 ¹⁴	1.34 x 10 ¹⁵

Fig. 1. Structural model for capacitive pressure sensor

B. Theory of operation of the square deflection and maximum stress

For a two dimensional diaphragm with a pressure load, p , the differential equation for the displacement of the diaphragm can be derived by analyzing the balance conditions for forces and bending moments in an elemental area of diaphragm, $dx dy$. The general equation for displacement $w(x, y)$ is found to be the differential equation of diaphragm for displacement is given as equation (1), where we measure the point at the center of the diaphragm due to pressure applied on its surface:

$$D \left[\frac{\partial^4 w}{\partial x^4} + 2 \frac{\partial^4 w}{\partial x^2 \partial y^2} + \frac{\partial^4 w}{\partial y^4} \right] + h \rho \frac{\partial^2 w}{\partial t^2} = p(x, y) \quad (1)$$

This equation is based on time dependence, so it can be used for frequency analysis. D is the flexural rigidity, h is the diaphragm's thickness and ρ is density of the diaphragm material. If the pressure p is uniform then the steady displacement can be expressed as equation (2):

$$D \left[\frac{\partial^4 w}{\partial x^4} + 2 \frac{\partial^4 w}{\partial x^2 \partial y^2} + \frac{\partial^4 w}{\partial y^4} \right] = p \quad (2)$$

For a square diaphragm with a side length of $2a$ as shown in Figure 2, the simplest expression of displacement for a pressure p can be expressed by equation (3) [5]:

$$w(x, y) = \frac{1}{47} p \frac{a^4}{D} \left(1 - \frac{x^2}{a^2} \right)^2 \left(1 - \frac{y^2}{a^2} \right)^2 \quad (3)$$

Fig. 2. Structure geometries of a square diaphragm

Since the deflection of the diaphragm is higher than its thickness, the strain in the middle plane of the diaphragm could be neglected. Thus the diaphragm stresses as well as the maximum stresses components for normal stress on surfaces perpendicular to x axis (σ_x) and normal stress on surfaces perpendicular to y axis (σ_y) were considered. The equations for diaphragm stresses are as follows equation(4) and (5):

$$\sigma_x = - \frac{E}{1-\nu^2} \left[\frac{\partial^2 w}{\partial x^2} + \nu \frac{\partial^2 w}{\partial y^2} \right] - \frac{E \alpha \Delta T}{1-\nu} \quad (4)$$

$$\sigma_y = - \frac{E}{1-\nu^2} \left[\frac{\partial^2 w}{\partial y^2} + \nu \frac{\partial^2 w}{\partial x^2} \right] - \frac{E \alpha \Delta T}{1-\nu} \quad (5)$$

Note that E is Young's modulus, ν is Poisson's ratio of the diaphragm material, w is vertical deflection of the diaphragm, α equal to $\epsilon/\Delta T$, where ϵ is strain and ΔT is temperature change with respect to reference temperature.

III. SIMULATION AND RESULTS

A. Simulation Settings

CoventorWare ver.2008 simulation software is used in this research to design, simulate and modify the performance of MEMS capacitive pressure sensor. It has three main components: Architect, Designer and Analyzer [6]. Architect is used to design the schematic of the capacitive pressure sensor. Designer is used to build the 3D design of the diaphragm. Analyzer is used to analyze the diaphragm deflection with given pressure and temperature.

Si and 3C-SiC materials with their respected electrical and mechanical properties are used to simulate the movable diaphragm (top plate). The anode (top plate) and cathode (bottom plate) separation is set to be $3 \mu\text{m}$, and the range of applied pressures is between 0 to 100MPa. The design steps include selecting the substrate layer and wet etching of the backside of the substrate to create the membrane. The next process is mesh creation for the device that is essential to allow the Analyzer to do the pressure and temperature analysis. Both are performed using CoventorWare mechanical solver MemMech. Figure 3 and Figure 4 shows the diaphragm deformation and maximum stress under a series of different pressures, respectively.

Fig. 3. Deflection of diaphragm by applied pressure

Fig. 4. Maximum stress of diaphragm by applied pressure

Figure 5 shows the 3D model of the diaphragm using mapped bricks mesh generated by Designer [7]. There are three steps involved. Firstly is the substrate step, secondly is the silicon planar fill with an anisotropic front side wet etch, and thirdly Si/SiC top diaphragm by using stack material modeling action. The substrate layer material is silicon. The wet etch properties are 3 μm depth and 54.7° degree angle of the silicon substrate. The highest stress-deflection of the diaphragm for an applied pressure of 100MPa is at the center of the diaphragm. The resulting diaphragm stress-deflection at 3 μm considered as the touch-mode deflection. But in this paper, we are focuses on the deflection of the diaphragm only.

Fig. 5. 3D diaphragm model using mapped brick mesh with relevant boundary conditions.

B. Results and discussion

The capacitive pressure sensor is subjected to a range of temperatures namely 27°C, 300°C, 700°C and 1000°C. The reference temperature is at 27°C, where we assume that the diaphragm is stress free. It is also assumed that by heating the

diaphragm rapidly, the deflection is achieved without relaxation. Symmetric boundary conditions have been chosen for the planes at $x = 200\mu\text{m}$ and $y = 200\mu\text{m}$, where the pressure is applied at the center of the diaphragm.

Fig. 6. Deflection at differential pressures and temperatures with the diaphragm thickness of 1 μm

TABLE II:
LINEAR REGRESSION ANALYSIS FOR DEFLECTION RESULTS AT DIFFERENTIAL TEMPERATURES WITH THICKNESS OF 1 μm

Temperature (°C)	SiC		Si	
	Equation	R ²	Equation	R ²
27	$y=0.008x + 0.74$	1.00	$y=0.020x + 2.30$	1.00
500	$y=0.014x + 2.77$	1.00	$y=0.033x + 3.81$	0.87
700	$y=0.03x + 4.78$	1.00	$y=0.075x + 7.44$	0.98
1000	$y=0.043x + 7.38$	1.00	$y=0.122x + 16.54$	0.92

Figure 6 and Table II showed the deflection of the 1 μm diaphragm made of SiC and Si under a differential temperatures. At room temperature, the deflection at the center of the diaphragm for both SiC and Si increases linearity (R-squared value = 1.00) from 0-100MPa. It is observed that the elastic limit of both materials can sustain 100 MPa at room temperature.

However, this linear trend does not hold for Si at high temperatures. The deflection of Si diaphragm increases non-linearly for 500°C, 700°C and 1000°C with R-squared value at 0.87, 0.98 and 0.92, respectively. On the other hand, the deflection of the SiC diaphragm increases at high temperatures up to 1000°C, all with R-square value of 1.

The maximum deflection of the center of the diaphragm for SiC and silicon at 100MPa yields predicted result, where Si diaphragm deflects more compares to SiC diaphragm. At room temperature, the deflection for both Si and SiC diaphragm are 1.6 μm and 4.3 μm , respectively. At 1000°C, both Si/SiC diaphragms deflect 11.7 μm /28.4 μm , respectively. The Young modulus of SiC is approximately 3 times higher compares to Si, and hence, the SiC deflection is three time less [8]. It must also be pointed out that the silicon diaphragm shows non-linear deflection at high temperatures because of the stress due the stretching of the diaphragm [9]. In other words, Si diaphragm cannot sustain the loading pressure at such extreme environment.

For the capacitive pressure sensor to be used continuously over a long period of time, the diaphragm must be capable of responding to applied pressure and extremely temperature, and must retain its elastic property [10]. This analysis indicates that SiC diaphragm is indeed is much better suited for extreme environments than Si.

Fig. 7. Results of deflection at differential thickness of diaphragm at 500°C with thickness diaphragm of 0.05μm, 0.1μm, 0.2μm and 1.0μm

TABLE III

LINEAR REGRESSION ANALYSIS FOR DEFLECTION DIFFERENT THICKNESS AT 500°C

Thickness (μm)	SiC		Si	
	Equation	R ²	Equation	R ²
0.05	$y=0.062x + 4.43$	1.000	$y=0.091x + 7.32$	0.988
0.10	$y=0.042x + 4.09$	1.000	$y=0.076x + 6.87$	0.987
0.20	$y=0.038x + 3.70$	1.000	$y=0.063x + 6.33$	0.987
0.30	$y=0.020x + 3.50$	0.999	$y=0.032x + 6.11$	0.933
0.50	$y=0.017x + 3.23$	0.999	$y=0.027x + 5.70$	0.949
1.00	$y=0.014x + 2.77$	0.998	$y=0.033x + 3.81$	0.873

Figure 7 and Table III show the diaphragm deflection at 500°C at the different thicknesses. As shown in equation (3), the deflection is inversely proportional to the thickness. Moreover, Si diaphragms have larger deflection (16.96 μm) compare to SiC diaphragm (10.66 μm) at the thickness of 50nm. More importantly, the SiC diaphragm has more linear deflection compares to Si diaphragm at all thicknesses, as shown in Table III. We also observe the mechanical failure of Si diaphragm at 1000°C, which is due to the degradation of the surface of SiC diaphragm [11]. On the other hand, show consistent linearity throughout different thicknesses at such high pressure and temperature as recorded in Table III. It implies that very thin diaphragm below 1 μm of the capacitive pressure sensor should be use SiC material indicating a very high mechanical strength of the diaphragm that can able to survive a very high pressure and temperature without fracture [12]. These deflection results are useful in real fabrication practical applications by specified the parameter of the diaphragm.

Fig. 8. Results of maximum stress at differential temperature with the thickness diaphragm for 0.2 μm

TABLE IV

LINEAR REGRESSION ANALYSIS FOR MAXIMUM STRESS AT DIFFERENT THICKNESS AT 500°C

Temperature (°C)	SiC		Si	
	Equation	R ²	Equation	R ²
27	$y=5x - 15$	1.000	$y=7.098x - 13.2$	0.998
500	$y=5x + 150$	1.000	$y=7.643x + 168.7$	0.981
700	$y=10x + 400$	1.000	$y=12.13x + 480.2$	0.985
1000	$y=12.5x + 575$	0.996	$y=18.92x + 531.2$	0.959

The mechanical characterization to investigate the maximum stress on the diaphragm is performed using “Mises Stress” simulation. Figure 8 and Table IV show the maximum stress of a 200 nm thick diaphragm at the temperatures of 27°C, 500°C, 700°C and 1000°C. In theory as shown in equation (4) and (5), the stress diaphragm is proportional to the pressure and temperature. The stress distribution increases with the increment of pressure and temperature, however the stresses are less by using SiC material compare to Si. The temperature shows a significant influence of the diaphragm on the stress state.

The main point from Figure 8 is the fact that the SiC diaphragm has more linear stresses versus pressure as compares to Si diaphragm at all temperatures, as shown in Table IV. Amazingly, even at 1000°C the SiC diaphragm shows linear graph (R-squared = 0.996), which Si diaphragm shows a non-linear maximum stress (R-squared value = 0.959).

These results show that the maximum stress of the SiC diaphragm at 1825 MPa is much below the yield strength of the SiC material at 3440 MPa. Similarly, the maximum stress for silicon diaphragm is 2000 MPa, whereas the yield strength for silicon is 2673 MPa [13]. Further analysis will be carried out to investigate this finding.

IV. CONCLUSION

This paper simulates and compares the performances of a parallel-plate model of a pressure sensor, where the top movable plate is made of either 3C-SiC or Si. The movable square diaphragm has the area of 400 μm² with six different thicknesses (0.05, 0.1, 0.2, 0.3, 0.5 μm and 1.0 μm). The

mechanical stress-deflection is performed by loading high pressure and temperature up to 100 MPa and 1000°C, respectively. The 1 μm thick SiC diaphragm exhibits close linearity graph with R-squared value of 1, and the maximum deflection of 11.7 μm , whereas the Si diaphragm of the same thickness exhibits non-linear behavior with R-square value of 0.92, and maximum deflection of 28.4 μm at the applied pressure and temperature of 100MPa and 1000°C, respectively. SiC diaphragm consistently shows better linearity (in term of R-square values) over Si diaphragm with the stress simulation as well. The 200 nm thick diaphragm shows the R-square value of 0.996 at the extreme temperatures and pressures. Finally, it is shown that the maximum stresses of both SiC and Si are lower than the yield strength of both materials.

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