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Design and Optimization of Piezoelectric Pressure Sensor with AlN as piezo electric material for High-Temperature Application using COMSOL 5.3

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Abstract: Dynamic pressure sensors in contrast to static pressure sensors measure pressure changes in liquids or gases generated due to a blast, a propulsion or an explosion, where the temperature is normally high which is above 700°C[1]. Piezoelectric pressure sensors with their inherent advantage of direct transduction capability are drawing attention for high-temperature applications. Lead Zirconate Titanate (PZT) and Zinc Oxide (ZnO) are popular ferroelectric materials for Piezoelectric sensor applications. Aluminum Nitride (AlN) is a suitable candidate for high-temperature applications with its high melting point of 2673 K, the piezoelectric property remaining stable even up to 1423K, the energy band gap of 6.2eV, piezoelectric coefficient d33 of 7pC/N and pressure handling capacity up to 10 MPa. In this study, COMSOL Multiphysics 5.3 was used to analyse the pressure sensing capability of AlN film by optimizing the crystal orientation and the dimension of AlN in addition to studying suitability of using at high temperature. Also a comparison is done on the high temperature performance of pressure sensor using Silicon and Silicon Carbide as diaphragm.

Keywords: Sensor, Piezoelectric, Temperature, Aluminium Nitride, Pressure

1. Introduction

Pressure sensors are realized using piezoresistive, capacitive, fibre optic and piezoelectric principles. Piezoresistive sensors have the drawback of temperature-dependent resistance variation which leads to error in measurement at high temperatures. Capacitive sensors lack robustness and are prone to parasitic capacitive effects though they have better stability against thermal drift. The performance of fibre optic sensors is much dependent on packaging of the optical components for high-temperature operation with added cost on signal conditioning and processing. While dynamic pressure sensing requires piezoelectric sensing, new materials need to be identified for high-temperature MEMS based applications. As automation and autonomous systems are flourishing in the automotive and aerospace industries, the need for sensors operating in adverse environment is increasing [1]. The piezoresistive pressure sensor is mostly used because of its high sensitivity and ease of mass production. But the electrical and mechanical properties of commonly used materials get degraded when the temperature increases beyond 120^{o}C [2]. Piezoelectric pressure sensor has several advantages like good frequency response and suitability to measure dynamic pressure. The advantages of using piezoelectric material in MEMS applications are low power requirements, and efficient voltage-deflection conversion. Piezoelectric effect is exhibited by materials with certain specific asymmetry in their crystal structure, found in some of the natural crystals, such as quartz or tourmaline. In addition, specially formulated ceramics can be created with suitable polarisation to make them piezoelectric. These ceramics have higher sensitivities than natural crystals. AlN is a suitable piezoelectric material for high temperature dynamic pressure sensing applications. The melting point of AlN is 2673 K with stable piezo electric property even up to 1423K. It has high energy band gap of 6.2eV and piezo electric coefficient, d33: 7pC/N. It can witstand pressure upto 10 MPa . These performance parameters are achievable if the crystal orientation of AlN thin films is highly z- axis oriented [3]. High piezo electric coupling can be achieved if the layers are oriented in (002) direction with columnar z-axis grains perpendicular to the substrate. Process optimization is always a challenge alongwith choosing suitable electrodes.

To design a MEMS based pressure sensor, where multiple processes are involved, it is essential to model the structure and the responses to optimise the fabrication process. Here, the influence of the material properties and dimensions are studied using simulations. The anisotropic properties and the constitutive equations[4] for the piezoelectric effect are modelled using COMPSOL Multiphysics 5.3. The study conducted are primarily on the effect of crystal orientation and temperature on the piezoelectric coefficient of AlN thin film. Further, the study was extended towards the choice of the pressure sensor structure and the choice of diaphragm materials. A comparison study is performed on the high temperature performance of the sensor using Si and SiC as the diaphragm.

2. Method

2.1 Material selection for piezoelectric pressure sensor

2.1.1 Piezoelectric material

Among the numerous piezoelectric materials used for various applications, only a few can be used for higher temperature applications. Lead zirconate titanate has high sensitivity and high piezoelectric coefficient but it is toxic and has limited operating temperature (~200 ∘C). Zinc oxide is another candidate but is not chemically stable and produce low output values[5].

Polyvinylidene fluoride (PVDF) has low thermal stability and is melting at 177 ◦C. Quartz has a low piezoelectric coefficient and limited operation temperature (573 ◦C). Monocrystal ZnO has excellent heat resistance but suffers from several disadvantages such as poor durability, being expensive, and low sensor output. Aluminum nitride is a MEMS compatible piezoelectric material offering high service temperature limit (1200°C) ,hazard free process,high elastic coefficient (young modulus :314 Gpa) ,good linearity to pressure (0.1-1.6Mpa),good frequency property (0.1-100Hz) [3, 6], low dielectric losses [7],high breakdown field,high chemical inertness,hardness (hardness:17Gpa) [8],does not require polling [9] and high melting point(2830°C) [1].

AlN has hexagonal wurtzite crystal structure forming a thermodynamically stable structure with nitrogen [10]. AlN crystal structure differs from the ideal wurtzite structure because of the following two reasons. First, the axial ratio c/a is 1.6 instead of 1.633 and then the parameter value is 0.385 instead of 0.375. The axial ratio is defined as the ratio of height to base length of tetrahedron where c/2 is the height of tetrahedron and a is the base length of a tetrahedron. U parameter describes the Al-N separation along the trigonal axis. In an ideal wurtzite structure, each atom forms four equal bonds tetrahedrally.

A decrease in axial ratio describes the compression of the tetrahedra along the c axis. This leads to distortion between aluminium and nitrogen bonds when compared to the regular tetrahedral arrangements. U parameter value differs from the ideal wurtzite structure describes an atom is displaced along the c axis towards the base of a tetrahedron. Figure 1 shows the crystal structure of aluminium nitride.

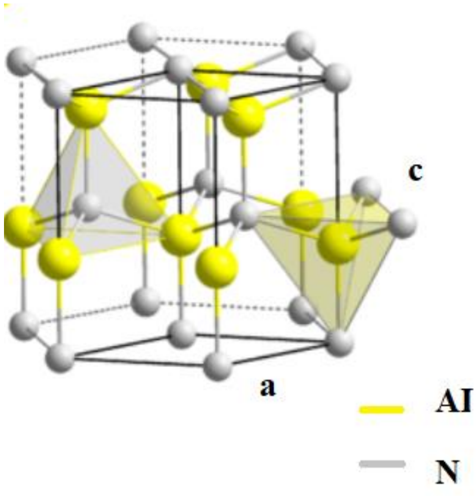

Figure 1. *Crystal structure for AlN*

2.1.2 Diaphragm Material

Silicon (Si) is used as a substrate for most of the sensors but its electronics property gets degraded above 250°C and mechanical properties get degraded above 600°C due to decrease in elastic modulus when the temperature gets increases. Silicon carbide (SiC) has good mechanical and thermal stability and also good electronic properties because of the wide bandgap. Some additional advantages of SiC are high chemical inertness and radiation resistance. And also single and polycrystal SiC can be grown on the large-area substrate. It is a one-dimensional polymorphism called polytypism. The difference in polytypes is only the stacking sequence of planes but all polytypes are an identical planar arrangement of silicon and carbon atom. The SiC has numerous crystal structures because of disorder in the stacking periodicity of the plane. A historically cubic, hexagonal, and rhombohedral phase of SiC is called alpha and beta SiC. But now cubic SiC as 3C-SiC, hexagonal phase of SiC as 2H-SiC,4H-SiC, and 6H-SiC. SiC polytypes have the same atomic composition but differ in electrical properties. Figure 2 shows that only the stacking sequence of the similar plane is varied for polytype. The bandgap for Silicon carbide ranges from 2.3 eV for 3C-SiC to 3.4 eV for 2H-SiC. SiC is etched by alkaline hydroxide and acid is not mostly used for etching. Silicon carbide does not melt but sublimes at 1800°C [11, 12].

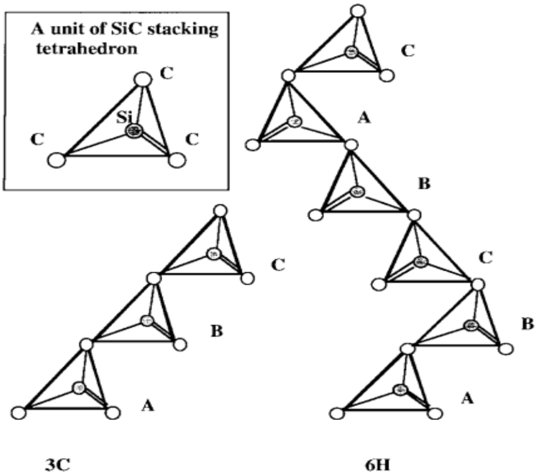

Figure 2. Stacking sequence of the plane [14]

2.1 3. Electrode material

The electrode should withstand high temperature and pressure. Molybdenum (Mo), Tungsten (W), and Titanium (Ti) have high creep resistance and strength even at high temperatures. Desired properties of the commonly used electrode materials are compared in Table 1. Tungsten has higher melting point than Mo and Ti but the tensile strength of Mo is high. Hence, Mo can withstand high pressure than W and Ti. Also, the elastic property of Mo is better than Tungsten and titanium. Electrical resistivity is low for molybdenum when compared to tungsten and titanium. The texture of Mo is softer than tungsten and also has high-temperature anti-oxidation, low coefficient of expansion, and long service life.

Table 1. Mechanical, electrical, and thermal properties of electrodes

Material	Poisson ratio	Tensile strength (MPa)	Young modulus (GPa)	Melting temperature (°C)	Electrical resistivity (ohm.m)
Tungsten	0.27	1670	340	3410	56E-9
Titanium	0.31	1654	689	1668	420E-9
Molybdenum	0.29	2620	217	2623	53.4E-9

2.1.3.1 Modelling using COMSOL Multiphysics

In COMSOL Multiphysics, solid mechanics and electrostatics are the two modules used for the piezoelectric pressure sensor analysis choosing stationary and frequency domain studies. Heat transfer module is used for temperature-dependency studies. Mutual coupling of the three physics(Solid mechanics, electrostatics and thermal) are performed for the study[13].

2.1.3.1.1 Geometry of the pressure sensor

The structure of piezoelectric pressure sensor consists of a substrate, piezoelectric active layer with top and bottom electrodes. Two models were studied with molybdenum electrodes. Silicon is used as the substrate etched to form the diaphragm in the first case and Silicon Carbide as the diaphragm in the second case as shown in figure 3 a and b. The pressure is applied at the bottom of the substrate.

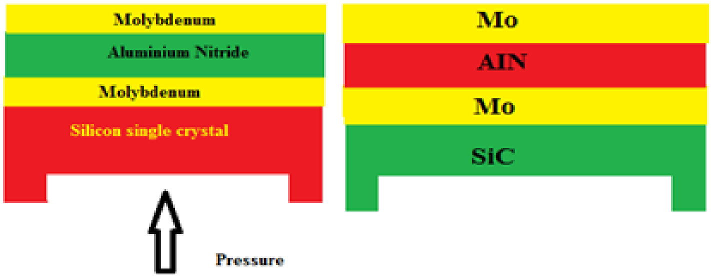

Figure 3. Structure of Piezoelectric pressure sensor

2.1.3.1.2 Materials

The materials used for the study are c-axis AlN, Mo, P-type single crystal Si and 6H-SiC. AlN was modelled using relative permttivity, density,compliance matrix, coupling matrix and elasticity matrix.Similarly, Si,SiC and Mo are modelled with elelctrical conductivity, density, thermal conductivity, Young's modulus etc.

2.1.3.1.3 Dimension

A preliminary optimization study was performed to choose the dimensions of the sensor along with the thickness of AlN, Mo and diaphragm. A square geometry of 1000μm side was chosen for the study.

2.1.3.1.4 Study

After modelling the materials, study was made on the performance of the pressure sensor in terms of electric potential with respect to varying temperature, maximum pressure handling capability. The design inputs were taken from the standard values of Kulite high temperature pressure sensor data sheet for the operating temperature, full scale output, natural frequency and maximum pressure[14]

3. Results and Discussion

3.1 C-axis AlN

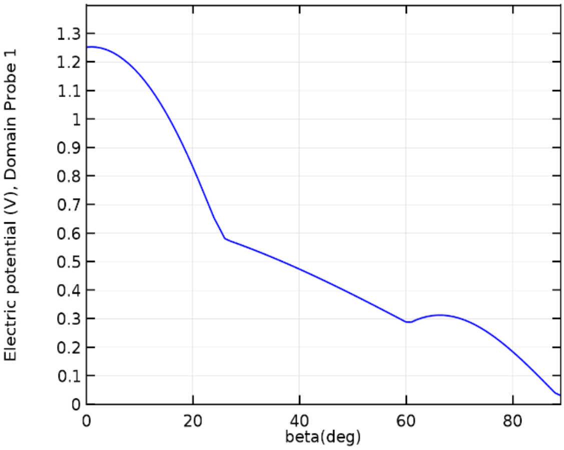

Figure 4. Euler angle (β)versus electric potential

To study the C axis orientation of the aluminium nitride rotated coordinate system is used. In the COMSOL Multiphysics environment, the most convenient way to specify a rotated coordinate system is through a set of Euler angles. The Euler angles required for a given crystal cut will vary for different orientations of the plate in the model global coordinates. The Euler angles determine the orientation of the crystallographic axes (X_{cr}– Y_{cr}–Z_{cr}) for the global coordinate system (X_g– Y_g–Z_g). Consequently, the orientation of the plate for the global system and the crystal cut determine the Euler angles. The Euler angles (α, β, γ) for z-axis orientation are 0,0 and 3.2 radian. β being 0° is z-axis orientation and becomes y-axis orientation at β equal to 90°. Figure 4 shows that electric potential decreases when Euler angle (β) increases. The z-axis orientation has high electric potential when compared to the y-axis orientation.

3.2 Temperature-Dependency Analysis

The Electric potential of the piezoelectric sensor under various temperature conditions is shown in figure 5 for c axis oriented AlN. The electric potential is constant up to 900°C. Above 900°C, the electric potential is greatly reduced and it reaches near to zero at 2000°C. This shows that the thermal stability of AlN is high compare to other piezoelectric materials. AlN can be used as the sensing element up to 900°C temperature.

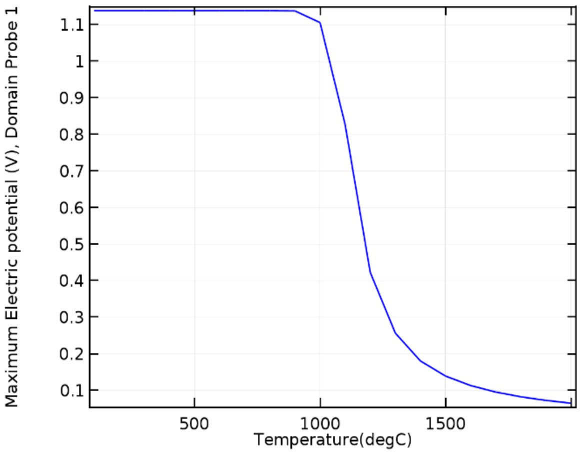

Figure 5. Electric potential of the piezoelectric sensor under various temperature conditions

3.3. Optimization of Piezoelectric Pressure Sensor Using Silicon As The Diaphragm

The electric potential and displacement for piezoelectric pressure sensor are shown in figure 6 and 7. The optimized dimensions of silicon substrate are 0.1x0.1x0.027cm and 0.5x0.5x0.05cm which produce electric potential of 1.01V and 1.96V as shown in Table 2. The pressure contact area is also an important factor and maximum pressure contact area for the 0.1x0.1x0.027cm and 0.5x0.5x0.05cm dimensions are 0.1x0.08 cm and 0.25x0.25cm.

Table 2. Optimization of the piezoelectric sensor using a silicon substrate

Sl. No.	(μm)	Thickness (μm)			Electric potential(V)	Pressure contact area (μm^2)
	Length and width	Silicon	AIN	Mo		
1	1000	500	1	0.1	0.32	1000X800
2	1000	270	1.4	0.1	1.01	1000X800
3	5000	500	1.4	0.1	1.96	2500X2500

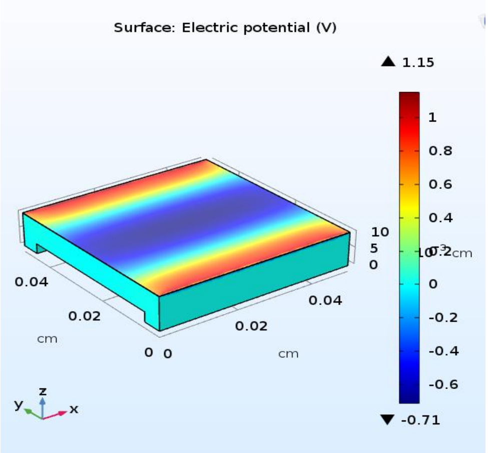

Figure 6. Electric potential for the piezoelectric pressure sensor

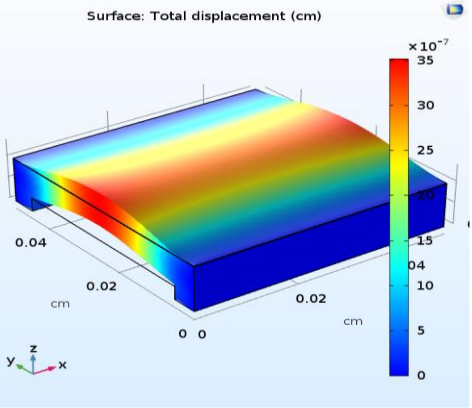

Figure 7. Electric potential for the piezoelectric pressure sensor

For the dimension 0.5x0.5x0.05cm, the pressure contact area should not exceed 0.25x0.25cm, otherwise, stress is higher than the tensile strength of the material and it may lead to damage. The tensile strength of the material is shown in table 3. The tensile strength of the silicon is higher than aluminium nitride and molybdenum.

Table 3. Tensile strength of the materials

Material	Single-crystal Silicon	AlN	Mo
Tensile strength(N/m^2)	2E^9	2.7E^8	3.24E^8

3.4 Optimization of piezoelectric pressure sensor using silicon carbide as a Diaphragm

Silicon carbide was used as the diaphragm and table 4 shows that the optimized dimension of the SiC is 0.1x0.1x0.016cm and 0.5x0.5x0.05cm which produce electric potential 1.64V and 1.49V, and its pressure contact area are 0.1x0.08cm and 0.5X0.4cm. Then comparing the simulation results of the piezoelectric sensor using silicon and silicon carbide as diaphragm was conducted considering the thickness of all the layers and their influence on the stress experience as shown in Figure 8. The stress experienced by Si, AIN, Mo bottom, and Mo top are lesser than their tensile strength even for substrate thickness below 300μm. The thickness of the silicon should be greater than 270μm, otherwise, the material will get a fracture.

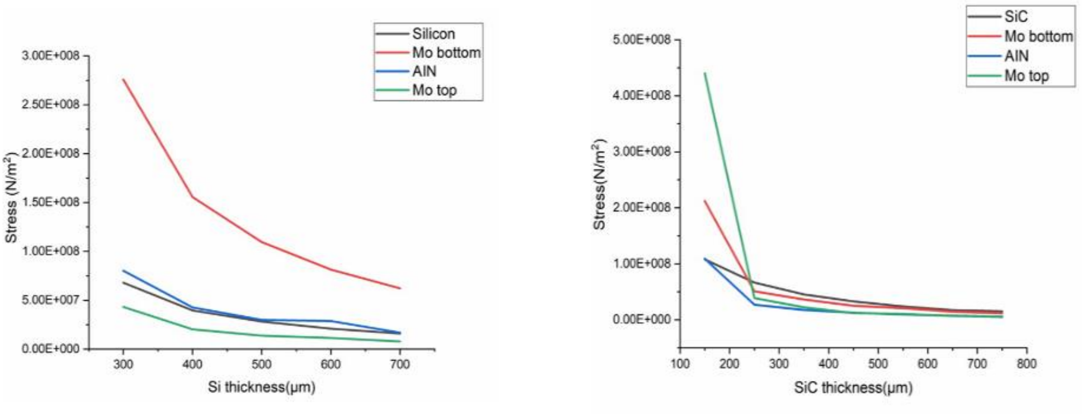

Figure 8. Effect of Layer thickness for Si and SiC device on the stress (2.6 MPa pressure limited by Mo bottom layer- optimized using Comsol for 1000 μm square)

Table 4. Optimization of the piezoelectric sensor using a silicon carbide substrate

		Thickness (µm)				
Sl. No.	Length and width (µm)	Si	AlN	Mo	Electric potential(V)	Pressure contact area (µm^2)
1	1000	500	1	0.1	0.07	1000X800
2	1000	160	1.4	0.1	1.64	1000X800
3	5000	500	1.4	0.1	1.49	5000X4000

The stress of SiC, AIN, Mo bottom, and Mo top is lesser than tensile strength even substrate thickness is reduced below 200µm as seen from Figure 8. The thickness of the SiC should be greater than 160µm, otherwise, the material will get a fracture. Figure 9 shows the maximum pressure which can be applied considering the withstandable stress of all the layers. The device with length of 1000µm, Si and Mo top can withstand the pressure is more than 7MPa but AIN and Mo bottom can withstand the pressure of 6.5 and 2.6 MPa. Thus, the maximum pressure limit is 2.6MPa. For a device of 1000µm using SiC diaphragm, Mo top can withstand the pressure of more than 20MPa but SiC, AIN, and Mo bottom can withstand the pressure of 6, 17, and 14 MPa respectively. Hence, the maximum pressure limit is 6MPa. The elastic property of silicon carbide is better than silicon because for the dimension SiC can withstand 6MPa but Si can only withstand 2.6MPa.

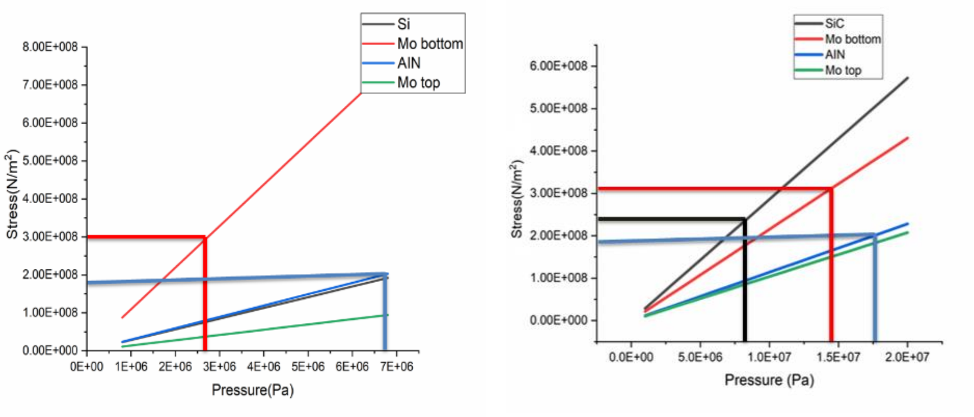

Figure 1. Maximum pressure applicable to Si and SiC pressure sensor considering the strength of electrode layers

The silicon carbide has better elastic properties and a large pressure contact area and it is suitable for high-pressure applications than a silicon substrate. The silicon and silicon carbide device was studied with the same dimensions of 0.1x0.1x0.05cm and produced 0.32V and

0.072V. But for the same dimension silicon produce high electric potential than silicon carbide and hence the silicon substrate is suitable for low-pressure applications because it produces high electric potential even for low pressure.

4. Conclusion

In summary, aluminium nitride produces stable output up to 900°C and it degrades when the temperature increases above 900°C. So AlN is used as a sensing element up to 900°C. The Z-axis orientation of AlN was modeled in COMSOL using a rotated coordinate system. In the study, Silicon was used as the diaphragm with molybdenum as electrodes and its dimensions were optimized using COMSOL Multiphysics 5.2. Further, a study was done using silicon carbide as the diaphragm. While optimizing the dimensions of the piezoelectric pressure sensor, the mechanical properties of all the layers of electrodes, diaphragm and the AlN were compared. The silicon carbide has better elastic properties and a large pressure contact area. It is suitable for high-pressure applications than a silicon substrate. Silicon substrate is suitable for low-pressure applications because it produces high electric potential even for low pressure.

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