Thermomechanical Study and Fracture Properties of Silicon Wafer under Effect of Crystal Orientation

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Abstract. Designing and optimizing the performance of a piezoresistive pressure microsensor involves not only studying the piezoresistive properties of polysilicon but also analyse the thermomechanical behaviour of its most sensitive internal part. This work focuses on an analytical, numerical and experimental study of a silicon wafer used in a pressure sensor. A thermomechanical study was conducted to assess the effects of temperature and material orientation on the deflexion and failure mode of Silicon membrane. The chosen analytical approach is based on Kirchhoff theory in which a square Silicon membrane is subjected to a distributed pressure over all its surface. Thermomechanical simulations and fracture analysis are carried out using Abaqus software. An experimental thermomechanical technique to determine maximum wafer deflexion and its effect on crack initiation and fracture mode was implemented. Deflexions tests were carried out on a bending machine using specimens of p-Si doped wafers. Deflexion values are measured for each applied temperature. Some preliminary tests were performed to determine the impact of temperature and Silicon wafers orientation on maximum deflexion when fracture occurs. The test’s results confirmed that the failure mode is highly brittle and follow each time crystal orientations 0° and 45°. Furthermore, at room temperature, fracture occur at 389 µm of displacement, and grows by 5.2 % when temperature is increased over 40°C. Consequently, Silicon sensitivity will be increased by 4%.

1. Introduction

The use of microsystems such as pressure sensors has increased due to their small size, high sensitivity and accuracy. Basically, there are two main classes of pressure sensors: piezoresistive and capacitive, but the principle of pressure detection has remained unchanged. To get the best design and quality of those devices, it shall simulate their behaviour to reduce additional development costs, its sensitivity and failure risks. The following section present a summary of the functioning principle of a Silicon piezoresistive pressure sensor with a brief theory background. The temperature dependency of thermal and mechanical properties such as expansion, conduction coefficients and Young’s modulus in the interval 20°C to 160°C are identified based previous publications [1] [2] [3]. A piezoresistive pressure sensor with movable diaphragm is composed mainly of an oxidized Silicon membrane covered with oxide as shown in figure 1. When a pressure is applied on the diaphragm, four piezoresistive polysilicon gauges placed over its top surface convert each mechanical deformation of the diaphragm into resistance variation. Sensor output is obtained by arranging gauges to form a Wheatstone bridge [4]. For designing and simulating the sensors, various aspects, such as fabrication technology, diaphragm thickness and orthotropic properties of silicon are considered. The applied pressure causes diaphragm deflection and stress to be measured by piezoresistors often placed in regions where high stress is generated. The
diaphragm thickness, shape, material orientation and mechanical properties as well as the piezoresistors orientation and location are important factors which affect the measured pressure.

Figure 1. Sectional drawing of a piezoresistive silicon-on-insulator membrane sensor.

The change in resistance of a piezoresistive material under stress is obtained by following equation:

$$\frac{\Delta R}{R} = \frac{\Delta L}{L} \frac{\Delta A}{A} + \frac{\Delta \rho}{\rho}$$

(1)

Where $\Delta L/L$ and $\Delta A/A$ are geometrical deformation regarding length and cross section of the resistors, respectively and $\rho$ is the resistivity.

These terms are negligible compared to $\Delta \rho/\rho$ in case of piezoresistors under stress [5]. Hence, the equation can be rewritten as follows:

$$\frac{\Delta R}{R} = \frac{\Delta \rho}{\rho} = \pi_1 \sigma_1 + \pi_2 \sigma_2$$

(2)

Where, $\pi_1$ and $\pi_2$ is longitudinal and transverse piezoresistive coefficients. $\sigma_1$ and $\sigma_2$ are the longitudinal and transverse stresses acting on the piezoresistor.

The piezoresistors are oriented along [110] directions on (100) wafer to maximize the piezoresistive effect. In Table 1, we present the piezoresistive coefficients for the transversal and longitudinal configurations of the gauges.

| Stresses direction | Current direction | Configuration | Piezoresistive coefficients | Piezoresistive coefficient | p-Si (resistivity =7.8Ω cm) |
|--------------------|------------------|---------------|-----------------------------|---------------------------|----------------------------|
| <110>              | <100>            | Longitudinal  | $\pi_1$                     | $\pi_1$                   | 6.6                        |
| <110>              | <010>            | Transversal   | $\pi_2$                     | $\pi_1$                   | -1.1                       |
| <110>              | <1-10>           | Transversal   | $(\pi_1 + \pi_{12} + \pi_{44})/2$ | $\pi_2$                   | 138.1                      |

2. Results and Discussion

2.1. Thermomechanical fracture simulation

A thermomechanical (TM) model of Silicon wafer fracture was developed using the finite element analysis (FEA). Finite element model of a Silicon wafer (diameter=50 mm, thickness=279 μm, crystal direction=100) is shown in figure 2-a. The central square surface is left free to apply pressure or concentrate force using a punch with a maximum descent speed of 0.5 mm/s. Initial temperature applied over the entire wafer is equivalent to the room’s temperature. The punch is a rigid body and its descent speed corresponds to that used in experimental tests. The Silicon wafer is held between two superposed male-female supports in order to leave free only the central square surface. Figure 2-b shows the ideal configuration of contact punch/wafer to analyse maximum deflexion propagation, fracture and stress distribution at various fixed temperatures. The test’s results confirmed that the failure mode is highly brittle and follow each time crystal orientations 0° and 45° [6]. These outputs are determined both by experimental tests and numerical simulation using FEA.
Figure 2. Finite element model of: a- the Silicon wafer; b- Contact configuration wafer/punch.

Preliminary tests indicate that fracture start at limit deflexion equal to 389 μm for a temperature of 100 °C. Finite element fracture simulations using a flat bottom punch confirmed the similar trends as shown in figure 3. To illustrate fracture propagation process, the punch course exceeds the limit requests of Silicon wafer. During the simulation tests, two wafers orientations are considered 0° and 45° according to direction <110>. Between these two orientations, mechanical properties varies by up to 45%.

(a) (b) (c)

Figure 3. FEA simulation and experimental of fracture. a- Fracture initiation; b- FEA fractured wafer: material orientation 45°, c- Experimental fracture for wafer oriented at 0°.

Figure 4 shows curves of maximum deflection versus temperature 20°C to 200°C. Both experimental and thermomechanical FEA (TM-FEA) are reported when Young’s modulus is equal to 130 GPa and 169 GPa respectively for chosen 0° and 45° orientations.

Figure 4. Variation of the deflection according to temperature.

2.2. Cristal orientation
The most common wafer type is called "(100) wafer", which means that the wafer’s surface is parallel to the silicon plane. According to <110> crystal direction, figure 5c shows typical directions X and Y in layout (100) for MEMS design [7]. The sample is placed in a well-defined orientation (plane 110) to ensure the correct positioning on the support. Young’s modulus and Poisson’s coefficient varies from 130 GPa to 169 GPa and from 0.28 to 0.36 respectively for one standard orientation at 0° to the maximum one at 45°[8]. Figure 5a and b present the variation of Young's modulus and the Poisson's coefficient according to crystal orientation 0° to 90° [9].
Figure 5. Mechanical properties variation at 0° and 45° crystal orientations. a- Young’s modulus (10^{11} \text{GPa}); b- Poisson’s ratio; c- Typical design orientation of Silicon wafers.

Most silicon wafers are not pure silicon; a certain amount of chemical impurities is usually added to control the electrical properties of the wafer. The volumetric effect of adding the mass of dopant atoms to the crystal lattice is negligible [10]. Since Young’s modulus variations can reach 45%, it was decreased by 10%, 20% and 30% respectively with respect to its average value, while leaving constant a same applied load equal to 25N. The corresponding displacement evolution is described in Table 2.

Table 2. Displacement rate evolution depending on variations of Young’s modulus and temperature.

| Temperature (°C) | Young’s modulus variations (%) | Displacement (%) |
|-----------------|--------------------------------|-----------------|
| 0               | 10                             | 3.09            |
| 50              | 20                             | 2.52            |
| 100             | 30                             | 2.37            |
| 200             | 10                             | 1.67            |
| 300             | 20                             | 1.31            |

By decreasing Young’s modulus values, displacement and stress will be increased consequently for the same applied load. However, increasing temperature generate opposite effect. It can be concluded that the direction of the plans must be respected to find the desired results.

The two piezoresistors (R1 and R3) are the longitudinal resistances, the variation of these two resistances can be calculated as follows [11]:

\[
\frac{\Delta R_1}{R_1} = \frac{\Delta R_3}{R_3} = \frac{\pi_{(110)} \sigma_{(110)} + \pi_{(110)} \sigma_{(100)}}{\pi_{44} \sigma_{(110)}} = \frac{1}{2} \pi_{44} (\sigma_{(110)} - \sigma_{(100)}) \approx \frac{1}{2} \pi_{44} \sigma_{(110)}
\]

(3)

The two piezoresistors (R1 and R3) are the longitudinal resistances, the variation of these two resistances can be calculated as follows [11]:

\[
\frac{\Delta R_2}{R_2} = \frac{\Delta R_4}{R_4} = \frac{\pi_{(110)} \sigma_{(110)} + \pi_{(110)} \sigma_{(100)}}{\pi_{44} \sigma_{(110)}} = \frac{1}{2} \pi_{44} (\sigma_{(110)} - \sigma_{(100)}) \approx -\frac{1}{2} \pi_{44} \sigma_{(110)}
\]

(4)

When the diaphragm is loaded, the longitudinal and transversal gauge resistors show opposite variations.

The variation of the output voltage with the loaded pressure is as follows:

\[
V_{\text{out}} = \frac{R_1 + \Delta R_1)(R_3 + \Delta R_3)(R_4 + \Delta R_4)}{R_1 + \Delta R_1 + R_3 + \Delta R_3 + R_4 + \Delta R_4 - \Delta R}
\]

(5)

Where the design meets perfect manufacture qualities, then R1 = R2 = R3 = R4 = R and ∆R1 = ∆R2 = ∆R3 = ∆R4 = ∆R. Output voltage can be rewritten as:

\[
V_{\text{out}} = I \times \Delta R = I \times \pi \times \sigma \times R
\]

(6)

The sensitivity of a pressure sensor is defined as the relative change in the output voltage per unit of applied pressure [12]:
Table 3 shows sensitivity variation for a temperature of 5°C to 100°C.

Table 3. The sensitivity temperature interval 5-100 °C.

| Temperature (°C) | Sensitivity (mV/V/MPa) |
|------------------|------------------------|
| 5                | 3.39                   |
| 25               | 3.48                   |
| 50               | 3.52                   |
| 75               | 3.61                   |
| 100              | 3.96                   |

3. Conclusion

In this article we have studied the influence of temperature and silicon crystal orientation on its thermomechanical behaviour and the maximum deflexion of a wafer used on piezoresistive pressure sensors. Two parameters were evaluated: the displacement of the diaphragm under different temperatures and the sensor sensitivity.

From 25°C to 80°C, the displacement variation was of 7.72%. On the other hand, it is 28.41% between 80 and 200°C. This variation is the result of the evolution of the coefficient of thermal expansion which changes by more than 50% between 25 and 150°C. This variation is the result of the evolution of the coefficient of thermal expansion which changes by more than 50% between 25 and 150°C [2]. In this case the sensor will be functional below 100°C.

Silicon wafer sensitivity was increased by 17% between 5 and 100°C, 2.65% between 5 and 25°C, 3.75% between room temperature and 75°C. Crack size and starting are proportional to temperature variation.

During room temperature experiments tests, fracture appeared for a displacement of 389 µm when a force of 25N was applied.

4. Références

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