Mathematical modeling of piezoresistive elements

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Abstract. This article presents the longitudinal piezoresistive coefficients for thin film amorphous semiconductor type a-C:H. Experimental data and mathematical models have been used in computer simulations. The results show that a reduction of the longitudinal piezoresistive coefficient occurs due to the increased concentration of impurities in the films analyzed.

1. Introduction
The focus of this work are the piezoresistive sensing elements based on thin film semiconductor type diamond like carbon - DLC obtained by a system of magnetron reactive sputtering. They are used traditionally known equations for the monocrystalline and polycrystalline silicon to determine the value of the piezoresistive coefficients, \( \pi \), amorphous DLC films and doped with nitrogen.

This paper presents the results of the piezoresistive effect for a film of hydrogenated amorphous carbon type (a-C:H/p-Si) with a nitrogen content ranging from 0% to 60%. These values are compared to models obtained by [1] into the monocrystalline silicon in which the impurity concentration values were obtained indirectly through mathematical simulations and experimental results given temperature range in the range 30 °C - 270 °C for film DLC [2].

2. Theory
The piezoresistive effect, \( \frac{\Delta \rho_{ij}}{\rho} \), is the change in electrical resistance, \( R \), of a semiconductor material when it is applied on a certain mechanical stress, \( T_{xy} \) given by equation (1).

\[
\frac{\Delta \rho_i}{\rho} = \sum_{j=1}^{6} \pi_{ij} T_j
\]  

The piezoresistive coefficients, \( \pi \), for P-type and N-type material are related to the levels of doping impurity concentration, the crystallographic orientation of the material, temperature and the type conductivity [1,6] data for the matrix of equation (2).

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In many cases, the mechanical stress, \( T_{ij} \), are components along the axis of the semiconductor crystal, but in other cases it works on an arbitrarily oriented coordinate system, so that the generalized Hooke's law should be used to determine the elastic deformation coefficients, \( S_{ijkl} \), expressed by equation (3).

\[
\varepsilon_{ij} = S_{ijkl} T_{ij}
\]  

(3)

Since, \( S_{ijkl} \) is a fourth order tensor constant elastic deformations of the substrate or film production considered for the sensor elements or diaphragms.

In matrix form, Equation (3) can be written according to equation (4).

\[
\begin{pmatrix}
\varepsilon_1 \\
\varepsilon_2 \\
\varepsilon_3 \\
\varepsilon_4 \\
\varepsilon_5 \\
\varepsilon_6 \\
\end{pmatrix} = \begin{pmatrix}
S_{11} & S_{12} & 0 & 0 & 0 & 0 \\
S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\
0 & 0 & S_{11} & S_{12} & 0 & 0 \\
0 & 0 & 0 & 0 & S_{44} & 0 \\
0 & 0 & 0 & 0 & 0 & S_{44} \\
0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix} \begin{pmatrix}
T_1 \\
T_2 \\
T_3 \\
T_4 \\
T_5 \\
T_6 \\
\end{pmatrix}
\]  

(4)

The piezoresistive coefficients and the mechanical stress can be converted to mechanical deformation by using the Young's modulus, \( E \), [3,4] according to equation (5).

\[
E = \frac{T}{\varepsilon}
\]  

(5)

Where, \( \varepsilon \) is the longitudinal elastic deformation of the test body (dimensionless).

In technical terms, numerically, load and pressure sensors can be described by equation (6).

\[
GF = \frac{\Delta R}{R_0}
\]  

(6)

The literature provides information on many of the properties of materials, however, it is up to the designer to evaluate and determine those that are important for a specific project. In this work were carried out reviews of relevant characteristics for a project of sensor elements for piezoresistive pressure transducers.

Mechanical sensitivity is changed mainly by the material resistivity, \( \rho \), mobility, \( \mu \), temperature, \( \theta \), and concentration of impurities, \( N \). The piezoresistance coefficients dependent on temperature and concentration of dopants. Therefore, the electrical properties of piezoresistores sensors are extremely sensitive to the presence of impurities, even in small concentrations [2]. Since the impurity concentration is given by equation (7).

\[
N = \frac{\rho}{q\mu}
\]  

(7)
The diagram shown in figure 1 shows how a semiconductor material behaves in electrical terms, mechanical and thermal [2]. From the analysis of these properties begins the design of a transducer.

![Diagram](image)

**Figure 1. Diagram "cross effects" in semiconductors.**

In addition to the dependencies represented in the diagram of figure 1, the sign and magnitude of the piezoresistive effect in semiconductor materials are associated with the dopant type, temperature, and quality crystallographic orientation [6].

3. **Features DLC films**

The diamond-like carbon films are amorphous materials with a structure in which carbon atoms bonds vary between graphite and diamond. These materials have unusual combination of electrical, optical, thermal and mechanical [7]. Its main properties are: hardness, high carrier density, low roughness, chemical and inherent possibility of being intrinsically produced, p-type and n-type with a band gap ranging from 0.5 eV to near 4 eV [8].

In addition to presenting high strength, the films a-C:H show good step coverage can be used as anti-corrosion barriers and have the advantage of being filed with low roughness and excellent uniformity over large areas [10]. But have disadvantages such as high voltage and low internal mechanical stability which can be minimized considerably through improvements in deposition techniques. These strongly influence the electrical characteristics of DLC films. Since only changing the temperature of deposition can vary the resistivity $10^6$ to $10^{16} \Omega \cdot cm$ [8].

The piezoresistive effect on DLC films can be defined as an agglomerated composition $sp^2$ erratically in an insulating matrix $sp^3$ as shown in figure 2. In this description, the agglomerates $\pi$ bonding energy with no local create conditions for $sp^2$ bonds form the first pair, and subsequently forming C-C bonds (ethylene). The recombinations of bonds then form hexagonal rings such as benzene. Following the masses become graphitic within the $sp^3$ matrix.

In figure 2, the size of the agglomerates is indicated by, $s$, which are relatively large and the distance between two clusters is indicated by, $d$, which is typical of quantum mechanical tunnelling.
Similarly, the model for many valleys silicon, where energy ellipsoids are deformed when a mechanical stress is applied this model to the a-C:H is observed that when a mechanical stress is applied to the piezoresistor, the value of distance between two clusters $sp^2$ increases and therefore the amount of piezoresistance also increases. Otherwise, when a compressive mechanical stress the distance between the clusters is being applied to reduce the value of this decrease is attached piezoresistance [2].

The piezoresistive effect described in this way follows the model that explains the sensitivity factor or "gauge factor" (GF) in thick film resistors [7], establishing the empirical relationship between the value of electrical resistance and sensitivity. The very resistive materials should have high GF values. Otherwise, the source of the piezoresistive effect on DLC films can be described as a composition $sp^2$ agglomerates unevenly in a $sp^3$ matrix insulator as shown in figure 2.

![Figure 2. Model for DLC films. (a) without mechanical and (b) with mechanical stress effort [2].](image)

As there are many similarities between the various DLC films used as piezoresistive elements can approach them to the models equivalent to those of silicon with cubic structure and shape the practical way of sensing element [2].

4. Mathematical model

It is noted that the sign and the magnitude of the piezoresistive effect in thin films associated with semiconductor dopant type, temperature, crystallographic orientation and quality [2,6]. Therefore, all of the physical properties of a material are dependent on the temperature so that the physical designs of piezoresistores must take this fact into consideration as shown in equation (8).

$$R(P, \theta) = R_{ref}(\theta) \left[ 1 + \pi_{xx}(\theta)T_{xx}(P, \theta) + \pi_{xy}(\theta)T_{xy}(P, \theta) \right]$$  \hspace{1cm} (8)

Where, $P$ is the applied pressure, $\theta$ is the temperature, $R_{ref}$ is no mechanical stress resistance at the reference temperature (300K), $\pi_{xx}$ piezoresistive coefficient is the shear in the xy plane and $T_{xy}$ is the average shear mechanical stress [2].

5. Results and discussions

Using the experimental data obtained by [2] for a film type a-C:H/Si/Ag with average resistivity, $\rho_{avg} = 4.22 \text{ M}\Omega\cdot\text{cm}$ was performed mathematical simulation to obtain the longitudinal piezoresistive coefficients for the film. The values were compared with films containing a nitrogen level which increase the field emission properties and reduce internal mechanical stress in the films.

The DLC films are characterized by having high resistivity values in a very wide range. Therefore, if they were designed with piezoresistor 2500 $\Omega$ typical resistance as is usual with mono and
polycrystalline silicon films, the films analyzed in current research should have an extraordinary level of doping as illustrated by the results shown in the next figures.

![Figure 3. Longitudinal piezoresistive coefficient for different DLC films (doped and undoped).](image)

The variation of the longitudinal piezoresistive coefficient is best observed at temperatures above 100 °C the films doped with 40 % and 60 % of nitrogen. In certain temperature ranges these doped layers have increasing linear behaviour and other decreasing this occurs because of changes that the dopant and the temperature produce the internal properties of the film. Therefore, the linear behaviour shown in Figure 3, the undoped DLC film, is according to the values suggested by the literature.

Figure 4 shows the function of the resistance value variation for doping the film a-C:H undoped (that is without any content of nitrogen) and temperature increases in the range of approximately 45 °C.

![Figure 4. Resistance as a function of variation of doping N in a-C:H undoped (label to the film without nitrogen content).](image)
Figure 4 shows the exponential function of the behaviour of the resistance variation in doping undoped DLC films, this behaviour is in agreement with what is suggested in the literature for undoped Si films compared with films analyzed in this study. There is also in figure 4 that depending on the manufacturing processes the piezoresistor tends to assume a constant average value of electrical resistance as suggested [2].

Figure 5 shows the resistance value of the film a-C:H doped with 40 % nitrogen and temperature increases in the range of 33 °C.

![Figure 5. Resistance as a function of variation of doping N in a-C:H doped with 40 % of nitrogen.](image)

The electrical behaviour of the film, shown in figure 5, is due to the changes caused by the incorporation of nitrogen. The appearance of the curve also varies with the temperature and compared to the results shown in figure 4, show a significant increase.

Figure 6 shows the resistance value in function of the variation of doping to the film a-C:H with 60 % nitrogen and which increases the temperature in the approximate range of 45 °C.
Comparing the values shown in figure 6 with Figure 4 clearly noticed an increase of the resistivity in the first figure. Now, when comparing these values with those shown in figure 5 it is evident the influence of the doping concentration in the resistance value of the material changes dramatically including the shape of the curve.

Because of this analysis it is up to the designer piezoresistors evaluate and determine the amount of doping ideas for a specific project.

The change in electrical resistance for the film a-C:H undoped, subject to mechanical stress parallel to the flow of electric current is called the longitudinal piezoresistive coefficient, $\pi_p$, and is being shown in figure 7.
The exponential behaviour shown in figure 7 for the longitudinal piezoresistive coefficient versus doping variation is characteristic for type semiconductor film undoped a-C:H. The longitudinal piezoresistive coefficient shown in figure 7 tends to assume a constant average value as it gradually increases the value of the doping concentration.

The behaviour of the piezoresistive coefficient, $\pi_I$, shown in figure 8 is the film a-C:H doped with 40 % of nitrogen.
Figure 8 shows a considerable increase in the value of the longitudinal piezoresistive coefficient in relation to figure 7 when comparing values of incorporating the dopant in the film.

Figure 9 shows the value of the piezoresistive coefficient, $\pi_p$, to the film a-C:H doped with 60% of nitrogen.

\[ -3 \times 10^5 \]
\[ -2 \times 10^5 \]
\[ -1.5 \times 10^5 \]
\[ -2 \]
\[ -2.5 \]
\[ -3 \]
\[ -3.5 \]

\[ 10^{10} \]
\[ 10^{12} \]
\[ 10^{14} \]
\[ 10^{16} \]
\[ 10^{18} \]

\textbf{Figure 9.} Longitudinal piezoresistive coefficient according to the N doping of variation for a-C:H doped with 60% of nitrogen.

It can be seen in figure 9 that the longitudinal piezoresistive coefficient has higher values when compared to figure 7 and figure 8. Therefore, it is evident that the nitrogen concentration significantly influences the piezoresistive coefficient of the material.

The results shown indicate that can be estimated with good precision the behaviour of a piezoresistive sensor element to be designed, although the values of the coefficients are relatively small.

6. Conclusion
This work shows that are needed new simulations to improve the models set to obtain the piezoresistive coefficients for thin film type doped DLC. It was observed that there is some coherence between the results obtained with those proposed in the literature. In many situations, particularly those in which the film is doped models proposed for crystalline films can be applied.

7. References
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