# CHAPTER 2

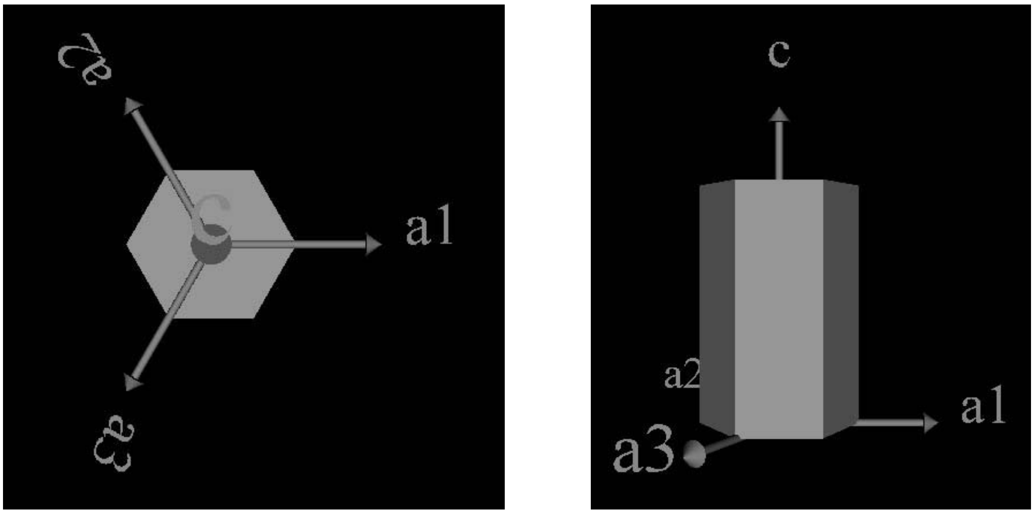
# MATERIAL PROPERTIES

PSOI and 6H-SiC substrate materials are used to make high temperature piezoresistive sensors in this study. In comparison with polysilicon, the properties of 6H-SiC have not been well documented. Therefore, in this chapter, elasticity and piezoresistivity of 6H-SiC will be reviewed and summarized. The isotropic material properties on the (0001) surface of 6H-SiC will be presented at the end of this chapter.

## 2.1 Crystal Structure of 6H-SiC

The crystal class of 6H-SiC is *6mm*, which belongs to the hexagonal crystal system. It has four indices in the Milller Index system as illustrated in Fig. 2.1. The representation of this system is [$a_1$, $a_2$, $a_3$, $c$]. To determine a space in the hexagonal crystal system, the three non-coplanar axes, $a_1$, $a_2$, $c$, are sufficient. So $a_3$ is a redundant variable in the hexagonal system representation and the following equation needs to be satisfied:

$$a_3 = \overline{a_1 + a_2}\ . \tag{2.1}$$



(a) (b)

**Figure 2.1. Miller Index system for a hexagonal system.**

The crystallographic structure of the hexagonal polytype 6H can be described by a series of one hexagonal and two cubic stacking layers (symbol **hcc**) with a hexagonal *c* axis for the hexagonal stacking layers and cubic [111] direction for the cubic ones. The atom stacking sequence of 6H-SiC is illustrated in Fig. 2.2.

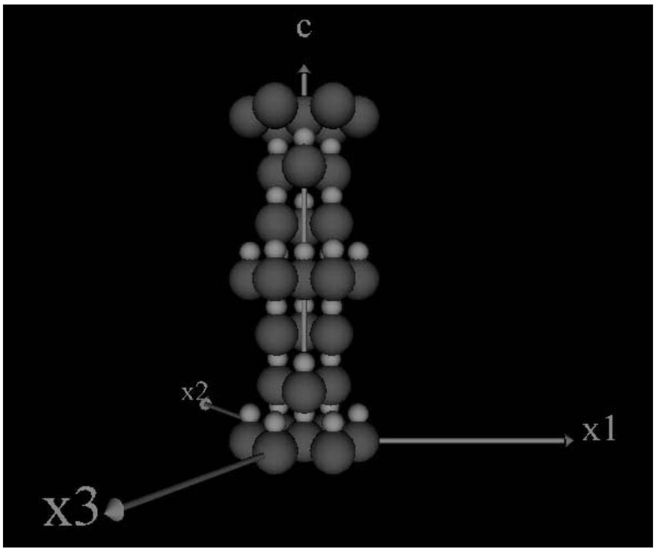


**Figure 2.2. Atom structure of 6H-SiC. Green (smaller) and blue (bigger) balls represent for carbon and silicon atoms, respectively.**

## 2.2 Elasticity and Piezoresistivity of 6H-SiC

The resistance of a material can be expressed by its geometry,

$$R = \rho \frac{l}{A} \tag{2.2}$$

where $l$ is the length, $A$ is the area and $\rho$ is the characteristic resistivity of the material. The derivation of the resistance can be expressed by

$$\frac{\Delta R}{R} = \frac{\Delta l}{l} - \frac{\Delta A}{A} + \frac{\Delta \rho}{\rho} \tag{2.3}$$

In this equation, if a stress is applied to the material, its geometry, resistivity and thus, resistance will be changed. Therefore, the expression in Eq. (2.3) can be written as

$$\frac{\Delta R}{R} = \varepsilon(1+2\mu) + \frac{\Delta\rho}{\rho} \tag{2.4}$$

where $\varepsilon$ is the strain which equals $\frac{\Delta l}{l}$ and $\mu$ is the Poisson's ratio.

The above derivation is based on an isotropic material, which means that the material's properties such as resistivity, Young's modulus, and Poisson's ratio are independent of the material's crystal orientation. For single crystalline semiconductor materials such as 6H-SiC, these properties depend on the crystal orientation and are anisotropic. The tensor expressions of the stiffness $\mathbf{c}$, compliance $\mathbf{s}$, and piezoresistance $\boldsymbol{\pi}$, of a semiconductor with hexagonal crystal structure have five independent variables which are connected by the following expressions.

$$\boldsymbol{\sigma} = \mathbf{c} \cdot \boldsymbol{\varepsilon} \tag{2.5}$$

$$\boldsymbol{\varepsilon} = \mathbf{s} \cdot \boldsymbol{\sigma} \tag{2.6}$$

$$\frac{\Delta\boldsymbol{\rho}}{\rho} = \boldsymbol{\pi} \cdot \boldsymbol{\sigma} \tag{2.7}$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are the tensor expressions of stress and strain, respectively. Because of the symmetry operation, the elastic stiffness coefficients, $c_{ij}$, the elastic compliance coefficients, $s_{ij}$, and the piezoresistance coefficients, $\pi_{ij}$, of the hexagonal crystal system can be written as

$$C = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{31} & c_{31} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} = {c_{11} - c_{12}}/{2} \end{bmatrix} \tag{2.8}$$

$$S = \begin{bmatrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{13} & 0 & 0 & 0 \\ s_{31} & s_{31} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{66} = 2(s_{11} - s_{12}) \end{bmatrix} \tag{2.9}$$

and

$$\Pi = \begin{bmatrix} \pi_{11} & \pi_{12} & \pi_{13} & 0 & 0 & 0 \\ \pi_{12} & \pi_{11} & \pi_{13} & 0 & 0 & 0 \\ \pi_{31} & \pi_{31} & \pi_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \pi_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \pi_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \pi_{66} = \pi_{11} - \pi_{12}) \end{bmatrix} \tag{2.10}$$

respectively[25].

In order to perform the design and simulation of the proposed sensors, the Young's Modulus, $E$, Poisson's ratio, $\nu$, and the longitudinal and transverse piezoresistance coefficients, $\pi_l$ and $\pi_t$, in the direction of an arbitrary unit vector $\vec{l}$ with the direction cosines, $(l_i, m_i, n_i)$, in the hexagonal crystal system have to be known. They are defined as:

$$E = 1/s'_{11} = 1/\left[(1-n_1{}^2)^2 s_{11} + n_1{}^4 s_{33} + n_1{}^2(1-n_1{}^2)(2s_{13}+s_{44})\right] \qquad (2.11)$$

$$\nu = -\frac{s_{12}{}'}{s_{11}{}'} = -\frac{l_3{}^2 m_3{}^2(s_{11}+s_{33}-s_{44}) - m_3{}^2(1-2l_3{}^2)s_{13} - (l_1 m_2 - l_2 m_1)^2 s_{12}}{(1-l_3{}^2)^2 s_{11} + l_3{}^4 s_{33} + l_3{}^2(1-l_3{}^2)(2s_{13}+s_{44})} \qquad (2.12)$$

$$\pi_l = \pi'_{11} = (1-n_1{}^2)^2\pi_{11} + n_1{}^4\pi_{33} + n_1{}^2(1-n_1{}^2)(\pi_{13}+\pi_{31}+4\pi_{44}) \qquad (2.13)$$

$$\pi_t = \pi'_{12} = n_1{}^2 n_2{}^2(\pi_{11}+\pi_{13}+\pi_{31}+\pi_{33}-4\pi_{44}) + (l_1 m_2 - l_2 m_1)^2\pi_{12} + n_2{}^2\pi_{13} + n_1{}^2\pi_{31}$$

(2.14)

In Eqs. (2.11)-(2.14), the transformation from the crystal axes to an arbitrary unit vector, $\vec{l}$, is given by direction cosines between two axes, which can be expressed in terms of Euler's angles as described in Eq. (2.15) and depicted in Fig. 2.3.

$$\begin{bmatrix} l_1 & m_1 & n_1 \\ l_2 & m_2 & n_2 \\ l_3 & m_3 & n_3 \end{bmatrix} = \begin{bmatrix} \cos\phi\cos\theta\cos\psi - \sin\phi\sin\psi & \sin\phi\cos\theta\cos\psi + \cos\phi\sin\psi & -\sin\theta\cos\psi \\ -\cos\phi\cos\theta\sin\psi - \sin\phi\cos\psi & -\sin\phi\cos\theta\sin\psi + \cos\phi\cos\psi & \sin\theta\sin\psi \\ \cos\phi\sin\theta & \cos\phi\sin\theta & \cos\theta \end{bmatrix}$$

(2.15)

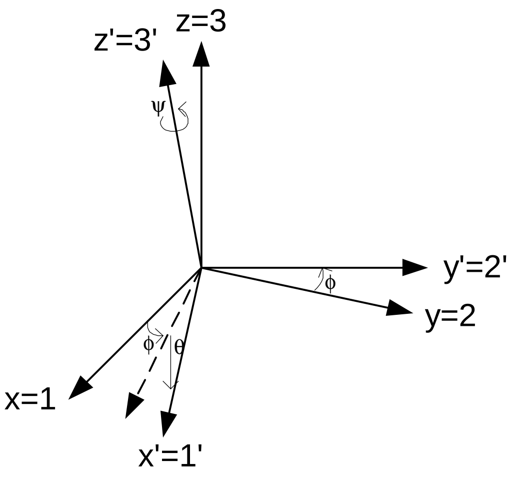


**Figure 2.3. Euler's angles.**

By Eqs. (2.11)-(2.14), the Young's Modulus, Poisson's ratio, and the longitudinal and transverse piezoresistance coefficient of a material with hexagonal crystal structure at any crystal orientation can be obtained if the elastic compliance and piezoresistance coefficients are known. For a (0001) on-axial 6H-SiC wafer, which is commercially available, the Young's Modulus, Poisson's ratio, longitudinal and transverse piezoresistance coefficient on the surface can be expressed as

$$E = 1/s_{11} \tag{2.16}$$

$$\nu = -s_{12}/s_{11} \tag{2.17}$$

$$\pi_l = \pi_{11} \tag{2.18}$$

$$\pi_t = \pi_{12} \tag{2.19}$$

Thus, they are independent of the crystal orientation on the (0001) surface of 6H-SiC wafers.

The four elastic constants $c_{11}$, $c_{33}$, $c_{44}$ and $c_{12}$ of 6H-SiC were first measured by Arlt and Schodder[26] by a resonance method and a double-pulse method. However, the complete set of elastic constants of 6H-SiC was published in 1997 by Kamitani and his co-workers[27] using the Brillouin-scattering method. The values of the elastic compliance and stiffness coefficients of 6H-SiC are rewritten in Table 2.1 and 2.2 according to Kamitani's results[27].

**Table 2.1. 6H-SiC elastic stiffness (unit: G Pa)**

| $c_{11}$ | $c_{12}$ | $c_{13}$ | $c_{33}$ | $c_{44}$ | $c_{66}$ |
|---|---|---|---|---|---|
| 501 | 111 | 52 | 553 | 163 | 195 |

**Table 2.2. 6H-SiC elastic compliance (unit: $10^{-11}$ $Pa^{-1}$)**

| $s_{11}$ | $s_{12}$ | $s_{13}$ | $s_{33}$ | $s_{44}$ | $s_{66}$ |
|---|---|---|---|---|---|
| 0.209 | -0.036 | -0.017 | 0.181 | 0.595 | 0.49 |

The reports of the piezoresistance coefficients of 6H-SiC can be traced back as early as 1968 by Rapatskaya[19]. Then, between 1974 and 1976, the Russian scientists Guk[28][29], Azimov[30] and Lomakina[31] also reported the piezoresistance coefficients of 6H-SiC with respect to different impurity concentrations and temperatures. Table 2.3 and 2.4 summarize the published results of n- and p-type 6H-SiC piezoresistance coefficients, respectively. In the tables, the gauge factors of 6H-SiC, which are derived by multiplying $\pi_{11}$ and $c_{11}$, vary significantly from each other due to different impurity concentrations and the varying quality of the SiC material, used by the authors. Because of the advance in 6H-SiC crystal growth technology, purer 6H-SiC wafers with larger size and fewer defects became commercially available. Shor and Okojie characterized the 6H-SiC piezoresistance coefficients with the doping concentration distributed between $10^{-17}$ and $10^{-19}$ cm$^{-3}$[20][32] and found that the magnitude of the gauge factor is about 30 at room temperature.

**Table 2.3. Published n-type 6H-SiC piezoresistive coefficients. (N.M.: No Mention)**

| **Year** | **Authors** | **Doping Level** cm$^{-3}$ | **Resistivity** Ω-cm | **Piezoresistance Coefficients** $\pi_{ij}$ (10$^{-11}$ Pa$^{-1}$) | **Gauge Factor** | **Reference** |
|---|---|---|---|---|---|---|
| 1968 | I.V. Rapatskaya,et al. | N.M. | 0.2 | $\pi_{11} = -7.8$<br>$\pi_{12} = -23.7$<br>$\pi_{13} = 32$<br>$\pi_{31} = -0.4$<br>$\pi_{33} = 0.8$ | -37 | [19] |
| | | N.M. | 2.5 | $\pi_{11} = -61.9$<br>$\pi_{12} = -1.08$<br>$\pi_{13} = 64.0$<br>$\pi_{31} = -26.9$<br>$\pi_{33} = 54.8$ | -295 | |
| | | N.M. | 23 | $\pi_{11} = -142.03$<br>$\pi_{12} = 26.0$<br>$\pi_{13} = 116$<br>$\pi_{31} = -26.9$<br>$\pi_{33} = 128.6$ | -676 | |
| 1974 | G.N. Guk, et al. | $1.7 \cdot 10^{17}$ | 0.45 | $\pi_{11} = -3.8$ | -18 | [28] |
| | | $1.6 \cdot 10^{18}$ | 0.12 | $\pi_{11} = -5.2$ | -25 | |
| | | $3 \cdot 10^{19}$ | 0.02 | $\pi_{11} = -2.7$ | -13 | |
| 1975 | S.A. Azimov, et al. | $3.0 \cdot 10^{17}$ | 1.1 | $\pi_{11} = -2.12$ | -10 | [30] |
| | | $2.9 \cdot 10^{17}$ | 0.63 | $\pi_{11} = -3.1$ | -15 | |
| | | $6.6 \cdot 10^{17}$ | 0.084 | $\pi_{11} = -6.0$ | -29 | |
| | | $8.3 \cdot 10^{17}$ | 0.18 | $\pi_{11} = -5.38$ | -27 | |
| | | $1.6 \cdot 10^{18}$ | 0.047 | $\pi_{11} = -8.33$ | -40 | |
| 1994 | J.S. Shor, et al. | $1.8 \cdot 10^{17}$ | 0.12 | $\pi_{11} = -7.2$ | -34 | [20] |
| | | $3.0 \cdot 10^{18}$ | 0.03 | $\pi_{11} = -6.02$ | -29 | |
| 1998 | R.S. Okojie, et al. | $2 \cdot 10^{19}$ | N.M. | $\pi_{11} = 5.3$ | 25 | [32] |

**Table 2.4. Published p-type 6H-SiC piezoresistive coefficients. (N.M.: No Mention)**

| Year | Authors | Doping Level cm$^{-3}$ | Resistivity Ω-cm | Piezoresistance Coefficients $\pi_{ij}$ ($10^{-11}$ Pa$^{-1}$) | Gauge Factor | Reference |
|---|---|---|---|---|---|---|
| 1976 | G.A. Lomakina | $5 \cdot 10^{20}$ | N.M. | $\pi_{11} = 10.5$<br>$\pi_{12} = -4.7$<br>$\pi_{13} = -8$<br>$\pi_{31} = -7.3$<br>$\pi_{33} = 23$<br>$\pi_{44} = 35$<br>$\pi_{16} = 2.5$ | 50 | [31] |
| 1998 | R.S. Okojie, et al. | $2 \cdot 10^{19}$ | N.M. | $\pi_{11} = 6.55$ | 31 | [32] |

Because on-axial (0001) 6H-SiC wafers will be used in this study, the isotropic model is used for the analytic model. The Young's modulus $E = 478$ GPa, the Poisson's ratio $\nu = 0.172$ and the longitudinal piezoresistance coefficient $\pi_l = \pi_{11} = 6.55 \times 10^{-11}$ Pa$^{-1}$ is used for the design of the piezoresistive pressure and tactile sensor. Due to the limited reference data, 500 MPa is used as the yield stress of 6H-SiC in order to obtain the working range of the piezoresistive sensors.