

Temperature-Dependent Elastic Constants of Substrates for Manufacture of Mems Devices

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ABSTRACT

We present a comparative computational study of temperature-dependent elastic constants of silicon (Si), silicon carbide (SiC) and diamond as substrates that are commonly used in the manufacture of Micro-Electromechanical Systems (MEMS) devices. Also mentioned is Cd₂SnO₄, whose ground-state elastic constants were determined just recently for the first time. Si is the dominant substrate used in the manufacture of MEMS devices, owing to its desirable electrical, electronic, thermal and mechanical properties. However, its low hardness, brittleness and inability to work under harsh environment such as high-temperature environment, has limited its use in the manufacture of MEMS like mechanical sensors and bioMEMS. The results show that the bulk modulus (B) is the most affected by temperature. Diamond recorded the highest decrease at 3.772%, while Si recorded the least at 2.070%. The shear modulus is the least affected, with Si recording a 0.359% and diamond a 0.821% decrease with increase in temperature.

I. INTRODUCTION

Silicon (Si) has been used as the substrate for the manufacture of Micro Electromechanical Systems (MEMS) devices for decades now. This owes to its unique properties such as electrical, mechanical and thermal, which are crucial for the application of MEMS. However, Si substrates are rigid, opaque and also have a limited area for processing (Patil, Chu & Conde, 2008). Thus, they are not ideal for the fabrication of transparent flexible MEMS devices such as sound transducers in air and water, in tactile sensors, and also in biomedical MEMS (bioMEMS) (Kim & Meng, 2019). Polymers have recently become alternatives to Si in the manufacture of MEMS devices due to their flexibility and transparency in the visible spectrum. Among the challenging tasks in working with polymers include their low melting point and poor electrical conductivity. This implies that they have to undergo the process of making them conducting, which is not economical. Moreover, they cannot be used to manufacture MEMS that operate under harsh environment such as high-temperature environment.

In a recent work, elastic constants of cadmium stannate (Cd₂SnO₄), a semiconductor that is transparent in the visible spectrum, was carried at the ground-state for the first time (Ongwen, Ogam & Otunga, 2020). The outcome of the study showed that Cd₂SnO₄ possesses desirable elastic properties that are comparable to those of Si. Moreover, the bulk modulus of Cd₂SnO₄ was found to be almost twice (150.3 GPa) compared to that of Si at 95 GPa (Kim, Cho & Muller, 2011), indicating that Cd₂SnO₄ is more incompressible compared to Si. The ductile nature of Cd₂SnO₄ obtained from the study (Ongwen, Ogam & Otunga, 2020), which implies that the material is easily deformed, also shades light into the possibility of having flexible and transparent MEMS fabricated on a semiconductor without any modifications. The objectives of this study were: (i) to compute the temperature-dependent elastic constants of Si, SiC and diamond; and (ii) to compare the temperature-dependence of elastic constants of Si, SiC and diamond in relation to their application as substrates in the manufacture of MEMS devices. The remainder of the paper is organized as follows: in section 2, the methodology that was used in carrying out the study is given. In section 3, the findings of the study are presented and discussed. In section 4, the conclusion derived from the results are given.

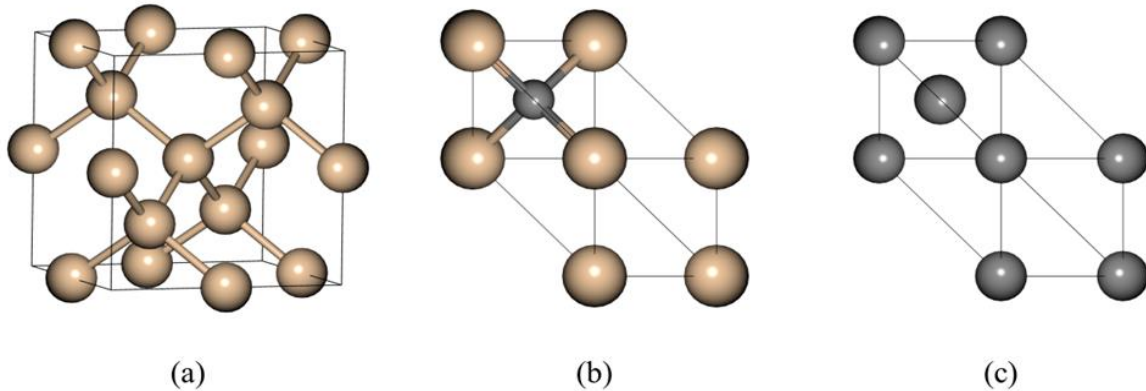
II. METHODOLOGY

The computation was performed using density functional theory (DFT) within the quantum espresso code. Simple cubic cells were used in all the calculations. For Si we used an Fd-3m cell with a space group number 227, consisting of 8 atoms. For both SiC and diamond, we used face-centered cubic cells (a space group number 225), both consisting of 2 atoms. For structural optimization, a variable cell relaxation was performed, which was done using the Brodyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm.

The equilibrium volume as well as the lattice points were obtained by minimizing the total energy. To determine the optimum lattice parameters, the equilibrium volume data were fitted using the third order Birch-Murnaghan equation of state. Figure 1 shows the structures of the three input files.

Figure 1

The Input Files For: (a) Si, (b) SiC and (c) Diamond. The Brown Balls Represent the Si Atoms, While the Grey Balls Represent the Carbon Atoms.



Calculation of the elastic constants of cubic crystals requires three elastic stiffness constants (c_{11} , c_{12} and c_{44}). The calculation of c_{11} , c_{12} and c_{44} at the ground state in this study was performed using stress-strain method, that is explained elsewhere (Ongwen, Ogam & Otunga, 2020). The stress-strain method has also been applied on orthorhombic phase of BaF₂ (Nyawere, Makau & Amolo, 2014). For the temperature-dependent elastic constants, we employed the quasi-harmonic approximation (QHA), which captures the effects of the entropy by factoring in the effects caused by thermal expansion. We made use of anisotropic expansion, which allows all the six lattice parameters to change without constraints. The anisotropic expansion model is more accurate in describing thermal expansion as compared to isotropic expansion, since most of the crystals exhibit some degree of anisotropy. The accuracy of the method is achieved by minimizing the argument over the crystal lattice vector $\mathbf{D}$, which defines the unit cell:

$$\mathbf{D} = \begin{bmatrix} D_1 & D_4 & D_5 \\ 0 & D_2 & D_6 \\ 0 & 0 & D_3 \end{bmatrix} \quad (1)$$

Application of strain to a system causes a change in the vibrational spectra of the crystal. There are two ways of computing the angular frequency ω for all values of $\mathbf{D}$. The first involves computing the mass-weighted Hessian for every structure with a unique lattice tensor $\mathbf{D}$. This is the most expensive step in the calculation. In the second step, an assumption is made that the changes in ω are proportional to the strains applied to the crystal, which is described by the Grüneisen parameter, which is a standard technique used to speed up lattice dynamics calculation (Abraham & Shirts, 2018). In the calculation of the anisotropic Grüneisen parameter, we treated the change in the vibrational frequencies as linear combination of changes in both the lattice vector and the volume of the cell. We calculated the anisotropic expansion using the formalism by Choy et. al., (1984), which is based on the probability of a strain (δ_i) placed on the lattice on the k^{th} vibrational frequency:

$$\partial(\delta_i)_{\delta_i \neq \delta_j} = \frac{(\partial \omega_k)_{\delta_i \neq \delta_j}}{\omega_k \lambda_{k,i}} \quad (2)$$

where δ_i is one of the six strains on the crystal matrix and $i = 1, 2, 3, \dots, 6$.

III. RESULTS AND DISCUSSION

Table 1 shows the ground-state values of elastic stiffness constants as well as the elastic constants for the three materials considered in this study, together with the values that are available in the literature. It is evident from the table that the calculated values of elastic constants in this study are in good agreement with those that are available in the literature. One striking factor here is the value of the Poisson's ratio of Cd_2SnO_4 . A value of below 0.27 implies that a material is brittle, while a value of more than 0.27 implies that the material is ductile. Thus, Cd_2SnO_4 is ductile while the rest of the substrates presented in this study are brittle, a property that is of great significance in the manufacture of flexible MEMS for various applications such as for bioMEMS.

Table 1

Ground-state Elastic Constants of Si, SiC, Diamond and Cd_2SnO_4 . B Is the Bulk Modulus, G Is the Shear Modulus, M Is the Poisson's Ratio, and E Is the Young's Modulus

	C_{11}	C_{12}	C_{44}	B	G	E	μ
Si	156.6	62.5	74.9	93.9	62.2	152.7	0.229
	165.6 ^(a)	63.9 ^(a)	79.5 ^(a)	97.8 ^(a)	65.2 ^(a)	130-169 ^(a)	0.26 ^(b)
SiC	387.5	139.3	243.9	222.0	186.0	436.0	0.172
	371.1 ^(c)	142 ^(c)	256 ^(c)	227 ^(c)		448 ^(d, e)	0.14 ^(d, e)
Diamond	1070.2	139.7	574.0	449.8	524.9	1138.2	0.078
	1076 ^(f)	125 ^(f)	576 ^(f)	443 ^(g)	577 ^(g)	1145 ^(g)	0.077 ^(g)
Cd_2SnO_4	278 ^(h)	125 ^(h)	83.1 ^(h)	150.3 ^(h)	53.7 ^(h)	143.8 ^(h)	0.341 ^(h)

(a) Experimental data from [Hopcroft, Nix & Kenny (2010)]

(b) Experimental data from [Hull, 1999]

(c) Data from [Dinesh et. al., 2015]

(d) Experimental data from [Mehregany, Zorman, Rajan & Wu, 1998] and [Mehregany et. al., 2000]

(e) Experimental data from [Spear & Dismukes, 1994]

(f) Experimental data from [Luo et. al., 2007]

(g) Data from [Papaconstantopoulos & Mehl, 2005]

(h) Computational data from [Ongwen, Ogam & Otunga, 2020]

Currently, there are no other data available in the literature on the elastic constants of Cd_2SnO_4 apart from our earlier work. Thus, there are no way of making a comparison of the data for Cd_2SnO_4 . However, the fact that the elastic constants of the other materials presented in table 1 are in very good agreement with those in the previous studies, gives confidence on the elastic constants of Cd_2SnO_4 obtained from the study. Figure 2 shows the elastic stiffness constants against temperature that were calculated using the QHA. It is evident from the figure that the elastic stiffness constants of all the three materials in this study decrease with an increase in temperature. The values of the elastic stiffness constants were used to calculate the elastic constants (bulk modulus, B; shear modulus, G; Poisson's ratio, μ ; and Young's modulus, E) (table 1) using the relations:

$$B = \frac{c_{11} + 2c_{12}}{3}, G = c_{44} - \frac{1}{5}[2c_{44} + (c_{12} - c_{11})] \quad (3)$$

$$\mu = \frac{c_{12} - \frac{1}{5}[2c_{44} + (c_{12} - c_{11})]}{2[c_{12} + c_{44} - \frac{2}{5}(2c_{44} + (c_{12} - c_{11}))]} \quad (4)$$

$$E = 2(1 + \mu)G \quad (5)$$

The decrease in elastic stiffness constants with temperature for the materials in this study has also been reported. Dinesh et. al. (2005) who studied the effect of temperature on elastic constants of SiC, also reported the decrease in all the three elastic stiffness constants. However, they reported a linear decrease in the elastic stiffness constants, unlike this study that observed non-linear relationship. The most likely reason for their observation is that all the three curves were drawn on the same vertical axis, although the value of c_{11} is much higher than those of c_{12} and c_{44} . A past study by Zouboulis et. al. (1998) investigated the temperature-dependent elastic stiffness constants of diamond. They found a non-linear decrease in the elastic stiffness constants with temperature, which agrees with

the outcome of the present study. Since the elastic constants of materials are derived from the elastic stiffness constants, the decrease in the elastic stiffness constants with temperature in this study implies a decrease in the elastic constants. All the three elastic stiffness constants c_{11} , c_{12} and c_{44} have almost equal sensitivity to temperature, since the slopes are almost equal in steepness. However, c_{12} is the most sensitive to temperature for Si and c_{11} for both SiC and diamond.

Figure 2

Temperature-dependent Elastic Stiffness Constants of Si, SiC and Diamond

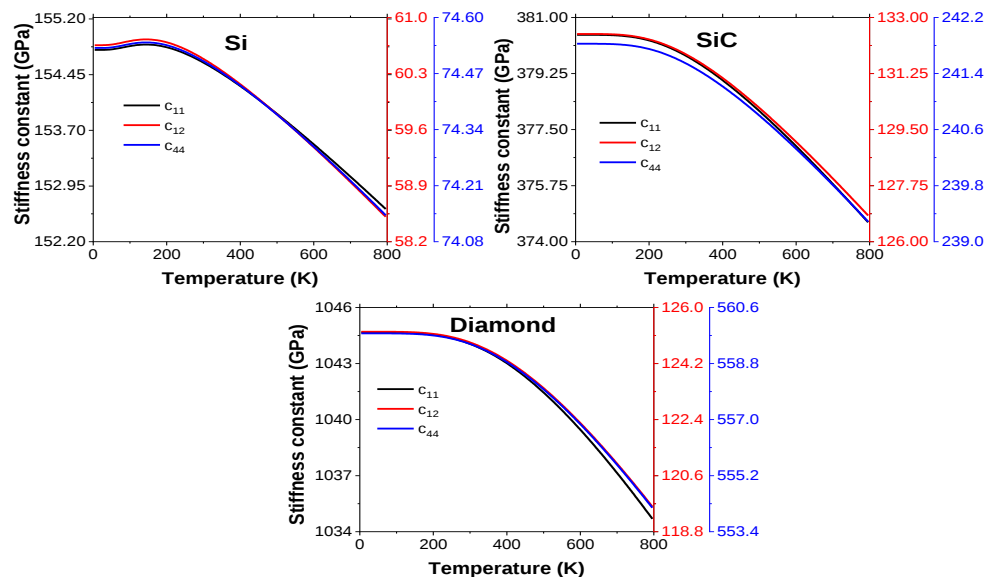
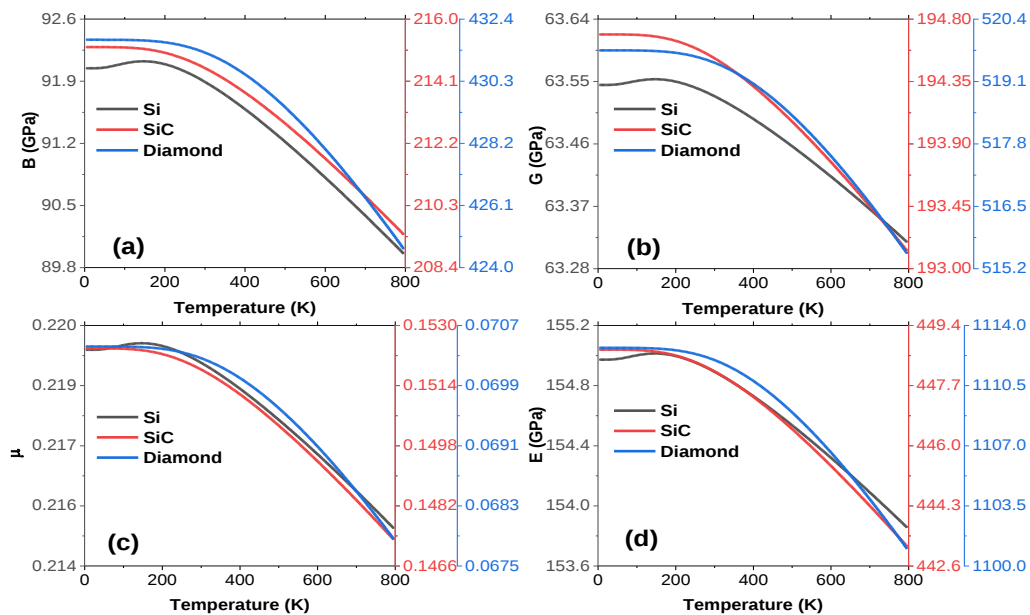


Figure 3 depicts the temperature-dependent elastic constants of the three materials. It is evident that the elastic constants of all the three materials decrease as the temperature increases. This agrees with previous studies on these materials, including the work by Zouboulis et. al. (1998). As can be observed in figure 3a, the curve for the bulk modulus of Si has a steeper slope than those of the other two materials. This implies that the bulk modulus of Si has the highest drop as temperature increases. The same observation is made for the Young's modulus of diamond (figure 3d)

Figure 3

Temperature-dependent Elastic Constants of Si, SiC and Diamond



Presented in table 2 is the percentage decrease in the four elastic constants of the three materials considered in this study. It is evident that both bulk modulus and Poisson's ratio are the ones most affected by temperature. The decrease in the Poisson's ratios implies that all the three materials become more brittle with increase in temperature. Diamond, which is the most brittle of all the three materials (table 1), recorded the highest decrease in the Poisson's ratio of 3.772%, while Si, which is the least brittle, recorded the lowest decrease at 2.070%. The high reduction of the bulk modulus of the materials with temperature implies that they become more vulnerable to fracture. SiC is the most affected of the three materials at 2.736%, while diamond is more likely to withstand fracture as the temperature increases (1.665%).

Table 2

Percentage Decrease in the Elastic Constants with Increase in Temperature in the Present Study

	B	G	E	μ
Si	2.322	0.359	0.726	2.070
SiC	2.736	0.808	1.254	2.942
Diamond	1.665	0.821	1.062	3.772

The shear modulus is the least affected of all the four elastic constants. This implies that all the materials maintain their rigidity as temperature increases. Si is the least affected at 0.359%, while diamond is the most affected at 0.821%. It is worthwhile to note that diamond is the hardest naturally occurring material, also called super hard material (Auciello et. al., 2004.). SiC recorded the highest decrease in the Young's modulus at 1.254%, while Si recorded the lowest at 0.726%. This implies that Si is most likely to resist longitudinal tension as the temperature increases, which is ideal in the fabrication of MEMS mechanical sensors as well as high-speed contact-mode micro-actuators, which are used in the fabrication of MEMS gears, micro engines rotors and accelerometers. Zouboulis et. al. (1998) reported an 8% decrease in the young's modulus of diamond in the temperature range of 300 – 1600 K. Although the value may not be very high; it is significant enough to cause a reasonable impact on the operation of a MEMS device. The report implies that diamond becomes less likely to resist longitudinal strain at higher temperatures above 800K that is considered in this study.

III. CONCLUSION

The comparison of temperature-dependent elastic constants of Si, SiC and diamond has been made. All the four elastic constants were found to decrease with increase in temperature. The properties most affected by temperature are the bulk modulus and Poisson's ratio, while the least affected property is the shear modulus. The bulk modulus of SiC is the most affected, while that of diamond is the least affected by temperature. For the shear modulus,

diamond is the most affected, while Si is the least affected. Diamond becomes the most brittle of all the three materials as temperature increases, while Si is the least, since the Poisson's ratio of diamond reduces the most, while that of Si reduces the least. Si is likely to resist longitudinal tension the most, since it exhibits the lowest decrease in the Young's modulus, while SiC is least likely to resist longitudinal tension.

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