



HAL
open science

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

Nicholas O. Ongwen, Erick Ogam, Henry Otunga, Zine El Abiddine Fellah,
Andrew Oduor, Maxwell Mageto

► **To cite this version:**

Nicholas O. Ongwen, Erick Ogam, Henry Otunga, Zine El Abiddine Fellah, Andrew Oduor, et al..
Temperature-Dependent Elastic Constants of Substrates for Manufacture of Mems Devices. Kabarak
Journal of Research & Innovation, 2022, 12 (1), pp.30. hal-04049864

HAL Id: hal-04049864

<https://hal.science/hal-04049864>

Submitted on 28 Mar 2023

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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

Nicholas ONGWEN¹, Erick OGAM², Henry OTUNGA¹, Z. E. A. FELLAH², Andrew ODUOR¹, Maxwell MAGETO

¹*Maseno University, P. O. Box Private Bag, Maseno, 40137, Kenya.*

Tel: +254 – 57 – 351620/22, Email: info@maseno.ac.ke

²*Laboratoire de Mécanique et d'Acoustique, LMA-UMR 7031 Aix-Marseille University-CNRS-Centrale Marseille, F-13453 Marseille CEDEX 13, France.*

Tel: (+33) 4 84 52 56 00, Email: lma[at]lma.cnrs-mrs.fr

³*Masinde Muliro University of Science and Technology, P. O. Box 190, Kakamega, 50100, Kenya*

Tel: +254 (0) 702597360, +254 (0) 702597361, Email: info@mmust.ac.ke

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. Mechanical sensors are fabricated on SiC and diamond due to their high Young's moduli as well as high fracture strength, while the bioMEMS are fabricated on polymers. The effect of temperature on the elastic constants of these substrates will help in giving insight into how their performance vary with temperature.

1. 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, 2016). 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 however, 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 can not be used to manufacture MEMS that operate under harsh environment such as high-temperature environment.

In a recent work, elastic constants of cadmium stannate (Cd_2SnO_4), 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 Cd_2SnO_4 possesses desirable elastic properties that are comparable to those of Si. Moreover, the bulk modulus of Cd_2SnO_4 was found to be almost twice (150.3 GPa) compared to that of Si at 95 GPa (Kim, Cho & Muller, 2011), indicating that Cd_2SnO_4 is more incompressible compared to Si. The ductile nature of Cd_2SnO_4 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.

2. The problem

Temperature is a factor that can greatly affect properties of materials. MEMS that operate under high-temperature conditions such as accelerometers and pressure sensors for airplane and underground oil exploration require thorough analysis of their behavior as temperature changes. Such MEMS have been fabricated on silicon carbide (SiC) and diamond. However, the two substrates are brittle and thus, not ideal for the fabrication of flexible MEMS. In this work, we present temperature-dependent elastic constants of Si, SiC and diamond obtained through *ab initio* calculation. The values of temperature-dependent elastic constant for Cd_2SnO_4 are still under study.

3. Objectives

The specific objectives of the study were:

- i. To compute the temperature-dependent elastic constants of Si, SiC and diamond
- ii. To compare the temperature-dependence of elastic constants Si, SiC and diamond in relation to their application as substrates in the manufacture of MEMS devices

5. Literature review

Ongwen, Ogam and Otunga, (2020) studied the elastic properties of Cd_2SnO_4 for the first-time using density functional theory. The outcome of the study showed that the elastic constants of Cd_2SnO_4 are comparable to those of Si. The bulk modulus was found to be almost twice as much as that of Si. One advantage of Cd_2SnO_4 over all the other substrates used in the manufacture of MEMS is that it is ductile, unlike the others that are brittle. The ductile nature of Cd_2SnO_4 was confirmed from both the Poisson's ratio as well as the Pugh's ratio.

Temperature-dependence elastic constants of doped Si has been reported (Ng et al., 2014). In the study, it was found out that the elastic constants of the resonators fabricated on the heavily doped Si were more sensitive to temperature than those that were lightly doped. Schall et al. (2008) also carried out a study to investigate the effect of temperature on elastic constants of Si using parametrization in the temperature range of 0 to 1200 K. The outcome of the study showed that crystalline Si showed a better trend in the elastic constants with temperature than the amorphous Si, both of which generally decreased with increase in temperature. Im, Park, Shin and Kim (2010) investigated the temperature-dependence of elastic constants of SiC using molecular dynamics, employing Tersoff's potential. Both the LAMMPS package as well as impulse excitation testing were used in the calculation of elastic constants. The study found out a

decrease in the Young's modulus of SiC from 475 to 425 GPa for a temperature range of room temperature to 1250 °C. The decrease in the elastic constants were recorded both in the experiment and in the simulation. A study by Xu et al. (2018) investigated the effect of temperature on mechanical properties of SiC. The calculation was performed using the VASP code. The outcome of the study showed that all the mechanical properties of SiC decreased with an increase in temperature from 300 to 1800 K, implying a softening behavior with temperature. They reported a 4.4% reduction in the Vickers hardness and a 7% reduction in the Young's modulus.

Magakubo, Ogi and Hirau (2016) studied the temperature-dependence of elastic constants of diamond. They found out that diamond possesses a high Debye temperature of about 2200 K and a small Gruneisen parameter of about 1. They concluded that these values show that diamond possesses small anharmonicity. In the study, the calculation of the elastic stiffness constants was performed using DFT. Gao et al. (2006) also studied the temperature-dependence of elastic constants at a temperature range of 100-1100 K by employing molecular dynamics as well as reactive empirical bond-order potential. The study found out that all the three elastic stiffness constants decrease with increase in the temperature. From the study, it was also found out that the bulk modulus decreased with increase in temperature. A past study by Zouboulis and Grimsditch, (1998) investigated the effect of temperature on elastic constants of diamond at a temperature range of 300 – 1600 K by applying Brillouin zone scattering. They found out that diamond is stable as temperature increases, as they recorded only a decrease in elastic constants of 8% for temperature rise of up to 1600 K. All the elastic stiffness constants decreased with increase in temperature.

From the previous studies, a comparison of the temperature-dependence of elastic constants of the substrates (Si, SiC and diamond) has not been made. The three materials are the dominant substrates currently being utilized in the manufacture of MEMS devices. This study thus provides a basis for choosing the most appropriate substrate to use for manufacture of different MEMS.

5. 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 (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.

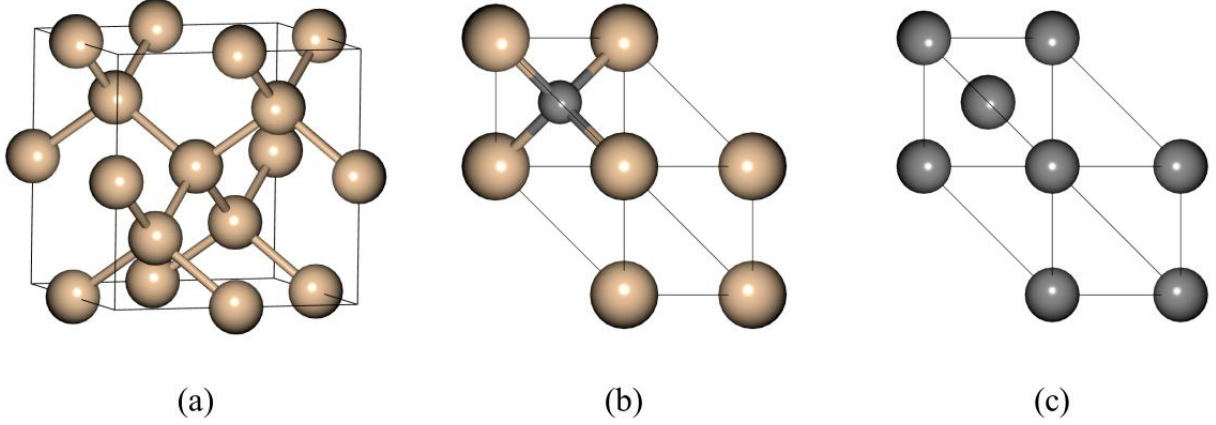


Figure 1: The input files for: (a) Si, (b) SiC and (c) Diamond. The brown balls represent the Si atoms, while the grey balls represent the carbon atoms.

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 and Otunga, 2020). 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 approximation. 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 and 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 $i = 1, 2, 3, \dots, 6$.

6. 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 of Cd_2SnO_4 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, μ is the Poisson's ratio and E is the Young's modulus

	c₁₁	c₁₂	c₄₄	B	G	E	μ
Si	156.6 165.6 ^(a)	62.5 63.9 ^(a)	74.9 79.5 ^(a)	93.9 97.8 ^(a)	62.2 65.2 ^(a)	152.7 130-169 ^(a)	0.2290 0.26 ^(b)
SiC	387.5 371.1 ^(c)	139.3 142 ^(c)	243.9 256 ^(c)	222.0 227 ^(c)	186.0	436.0 448 ^(d)	0.1720 0.14 ^(d)
Diamond	1070.2	139.7	574.0	449.8 443 ^(e)	524.9 577 ^(e)	1138.2 1145 ^(f)	0.0783 0.077 ^(e)
Cd_2SnO_4	278.0 ^(g)	125.0 ^(g)	83.1 ^(g)	150.3 ^(g)	53.7 ^(g)	143.8 ^(g)	0.3410 ^(g)

^(a)Experiment from [Hopcroft, Nix and Kenny (2010)]

^(b)Experiment from [Hull, 1999]

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

^(d)Experiment from [Mehregany, Zorman, Rajan and Wu, 1998] and [Mehregany et al., 2000]

^(e)Experiment from [Spear and Dismukes, 1994]

^(f)Experiment from [Luo et al., 2007]

^(g)Computation from [Ongwen, Ogam and 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 with any other previous work. 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 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) 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. (2015) who studied the effect of temperature on elastic constants of SiC, also reported the decrease in all the three the 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.

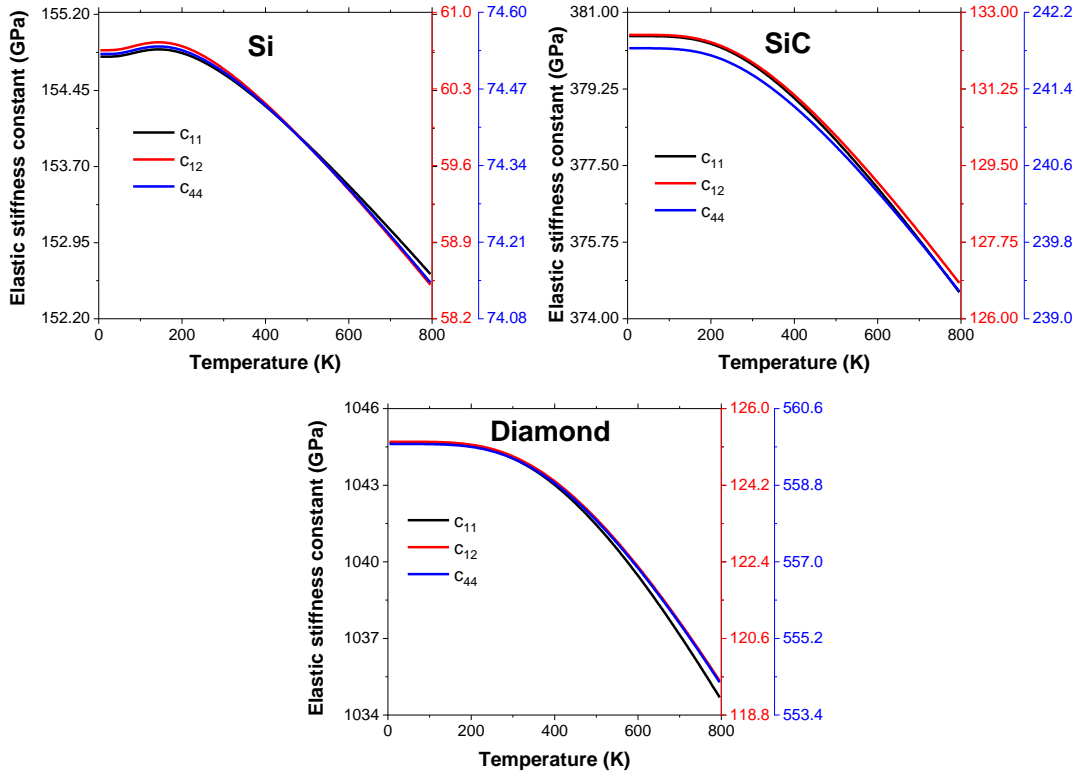


Figure 2: Temperature-dependent elastic stiffness constants of Si, SiC and diamond

Figure 3 discerns 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)

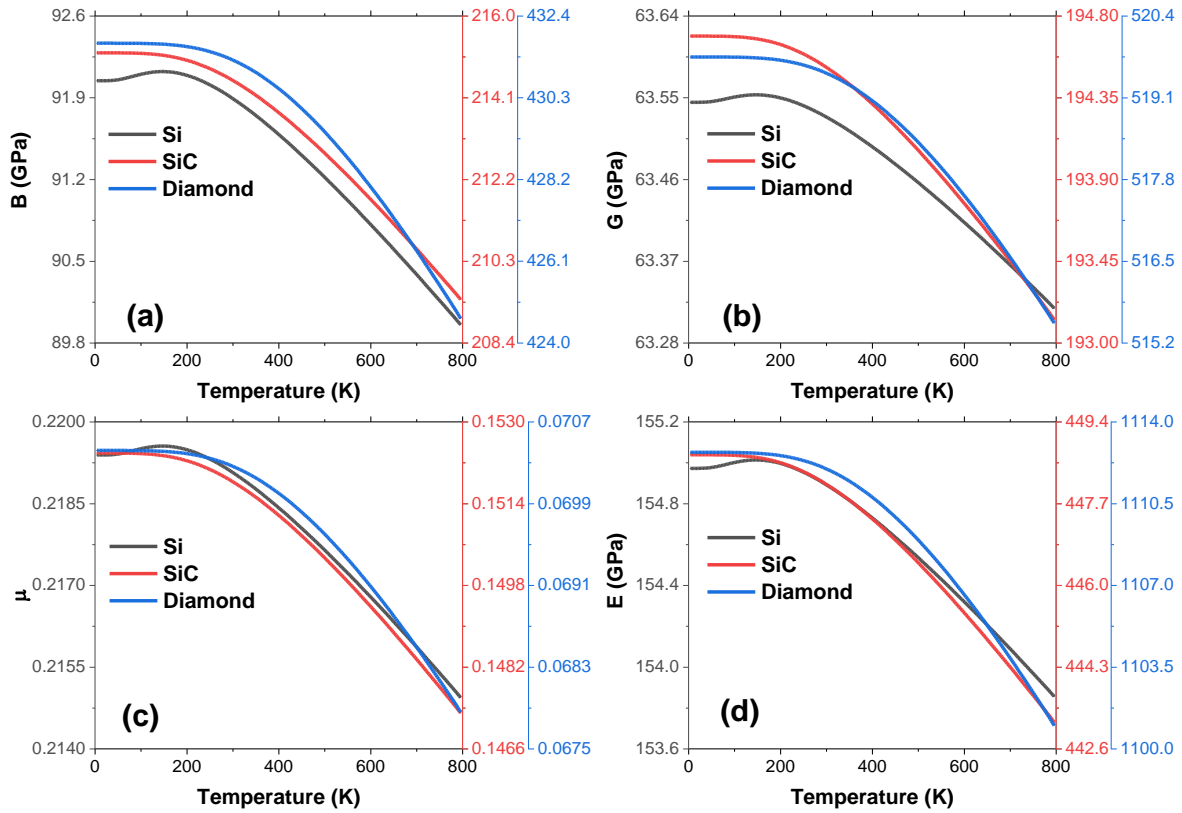


Figure 3: Temperature-dependent elastic constants of Si, SiC and diamond

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

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

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 (Lu and Chen, 2020). 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 e 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.

7. Conclusion

The comparison of temperature-dependent elastic constants of Si, SiC and diamond has successfully 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.

8. Recommendations

Apart from elastic constants, electrical and electronic properties of materials are also crucial properties of substrates that can greatly affect the operation of MEMS. Thus, research needs to be done on the effect of temperature on these properties.

Acknowledgement

The authors would like to sincerely appreciate the Centre for High Performance Computing (CHPC), South Africa for providing the computational resources that were used in the DFT calculations in this study.

References

1. Abraham, N., S. & Shirts, M., R. (2018). Thermal gradient approach for the Quasi-harmonic Approximation and its application to improved treatment of anisotropic expansion. *Journal of Chemical Theory and Computation (JCTC)*, **14**, 5904-5919. DOI: 10.1021/acs.jctc.8b00460
2. Aleksandrov, I., V. Goncharov, A., F. Stishov, S., M. & Yakovenko. (1989). Equation of state and Raman scattering in cubic BN and SiC at high pressure. *Journal of Experimental and Theoretical Physics*, **50**, 116.
3. Choy, C., L. Wong, S., P. & Young, K. (1984). Thermal expansion and Grüneisen parameters for anisotropic solids. *Physical Review B: Condensed Matter Materials Physics*, **29**, 1741.1747.
4. Dinesh, V. Shriya, S. Varshney, M. Singh, N. & Khenata, R. (2015). Elastic and thermodynamical properties of cubic (3C) silicon carbide under high pressure and high temperature, *Journal of Theoretical and Applied Physics*, **9**, 221-249. DOI 10.1007/s40094-015-0183-7.
5. Gao, G. Workum, K., V. Schall, J., D. & Harrison, A., H. (2006). Elastic constants of diamond from molecular dynamics simulations. *Journal of Physics: Condensed Matter*, **18**, S1737–S1750. doi: 10.1088/0953-8984/18/32/S05
6. Hopcroft, M., A. Nix, W., D. & Kenny, T., W. (2010). What is the Young's Modulus of Silicon? *IEEE Journal of Microelectromechanical Systems*, **19**, (2), 229-238. (DOI: 10.1109/JMEMS.2009.2039697).
7. Hull, R. (1999). *Properties of crystalline silicon*. London: INSPEC.
8. Im, j., I. Park, B-W. Shin, H-Y. & Kim, J-H. (2010). Temperature dependence on elastic constant of SiC ceramics. *Journal of the Korean Ceramic Society*, **47**, (6), 491-497. DOI:10.4191/KCERS.2010.47.6.491
9. Kim, B. & Meng, E. (2019). Review of polymer MEMS micromachining. *Journal of Micromachines and Microengineering*, **26**, 1-42.
10. Kim, J. Cho, D. & Muller, R. S. (2011). *Why is silicon (111) a better mechanical material for MEMS?* Seoul: Seoul National University.
11. Lu, C. Chen, C. (2020). Structure-strength relations of distinct MON phases from first-principles calculations, *Physical Review Materials*, **4** (4), 1-13.
12. Luo, J. K., Fu, Y. Q., Le, H. R., Williams, J. A., Spearing, S. M. & Milne, W. I. (2007). Diamond and diamond-like carbon MEMS. *Journal of Microtechnology and Microengineering*, **17**, 147-163
13. Mehregany, M., Zorman, C. A., Roy, S., Fleischman, A. J., Wu, C. H. & Rajan, N. (2000). Silicon carbide for microelectromechanical systems. *International Materials Reviews*, **45** (3), 85-108.
14. Mehregany, M., Zorman, C. A., Rajan, N. & Wu, C. H. (1998). Silicon carbide MEMS for harsh environments. *Proceedings of the IEEE*, **86** (8), 1594-1610.
15. Nagakubo, A. Ogi, H. & Hirao, M. (2016). Discussion on very small temperature dependence of diamond's elastic constants. *The Journal of the Acoustical Society of America*, **140**, 3203. <https://doi.org/10.1121/1.4970081>
16. Ng, E., J., Hong, V., A., Yang, Y. Ahn, C., H. Everhart, C., L., M. & Kenny, T., W. (2015). Temperature dependence of the elastic constants of doped silicon. *Journal of Microelectromechanical Systems*, **24**, (3), 730–741. doi:10.1109/jmems.2014.2347205
17. Ongwen, N., Ogam, E. & Otunga, H. (2020). Ab initio study of elastic properties of orthorhombic cadmium stannate as a substrate for the manufacture of MEMS devices. *Materials Today Communications*. <https://doi.org/10.1016/j.mtcomm.2020.101822>.
18. Patil, S. B. Chu, V. & Conde, J. P. (2008). Performance of thin film silicon MEMS on flexible plastic substrates, *Sensors and Actuators A*, **144**, 201-206.
19. Schall, J., D. Gao, G. & Harrison, J., A. (2008). Elastic constants of silicon materials calculated as a function of temperature using a parametrization of the second-generation reactive empirical bond-order potential. *Physical Review B*, **77**, 115209.

20. Spear, K. E. & Dismukes, J. P. (1994). *Synthetic diamond: Emerging CVD science and technology*. London: John Wiley and Sons Inc.
21. Xu, W-W. Xia, F. Chen, L. Wu, M. Gang, T. & Huang, Y. (2018). High-temperature mechanical and thermodynamic properties of silicon carbide polytypes. *Journal of Alloys and Compounds*, **768**, 722-732. doi: 10.1016/j.jallcom.2018.07.299
22. Zouboulis, E., S. Grimsditch, M. Ramdas, A., K. & Rodriguez, S. (1998). Temperature dependence of the elastic moduli of diamond: A Brillouin-scattering study, *Physical Review B*, **57** (5), 2889-2896.