Computation of Elastic Stiffness Constants, Elastic Moduli and Eigen Values of Stiffness Matrix of Some Crystals and Comparison with Experimental Results

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Abstract

This study computes the elastic stiffness constants of crystals α-Al_2O_3 and ZnO belongs to group of oxides, β-Si_3N_4 and h-BN belongs to group ofnitridesandSiC-4H, SiC-6Hbelongs to group of Carbides and its comparison with experimental results. Further, elastic moduli, eigenvalues of the stiffness matrix, the velocity of primary waves and shear waves in sample crystals along c-axis are computed using two different computational processes, viz., General Utility Lattice Program (GULF) and the ELATE Program. For the computation, the reported experimental data of cell parameters of sample crystals are used. The computed elastic stiffness constants of sample crystals are in close agreement with experimentally reported values. A high P- wave velocity of 13.52 Km/s is observed in β-Si_3N_4 indicating high stiffness, high density with low porosity. A high S- wave velocity of 7.22 Km/s is observed in SiC-6H, indicating SiC-6H is more rigid, dense and posses strong elastic properties. All the sample crystals, except ZnO have significantly high elastic moduli. This indicates excluding ZnO, the remaining crystals are highly thermodynamically and mechanically stable, stiffer with hardness and toughness nature. Poisson's ratio of α-Al_2O_3,ZnO, β-Si_3N_4 and h-BN are in the range of 0.2 to 0.35 where as it is low in the range of 0.15 to 0.17for SiC-4H and SiC-6H. Spatial variation of elastic moduli and Poisson's ratio of sample crystals are figured. The eigenvalues of stiffness matrix λ_1, λ_2, λ_3, λ_4 and λ_5 are high for SiC-6H compared to that of other sample crystals. Interestingly, λ_6 is high for h-BN compared to that of other sample crystals. Higher value of λ_6 of h-BN compared to other samples indicates that, h-BN is adequately constrained and therefore stable.

Key words: *carbides, elastic stiffness constants, elastic moduli, ELATE, GULF, nitrides, oxides*

1. Introduction

Elastic stiffness constants are very important parameters in crystals. They can provide information on stability, stiffness, brittleness and anisotropy of a crystal. Elastic constants also determines mechanical properties, structural stability, anisotropy, material design, wave propagation, modeling and simulation. They are closely correlated with thermal properties and phase transformation [1].The directional dependence of elastic constants and elastic moduli is a fundamental characteristics of most of the crystals and has significant implications in its practical applications in linear elasticity, the stiffness tensor relates stress to strain by Hooke's law. These constants are second order derivatives of the elastic energy density with respect to strain so that they encode how the crystal's internal energy changes under deformation [2].Elastic moduli determine a crystal's response to compression, shear and tension, enabling prediction of mechanical failure and ideal strength Bulk modulus measures a crystal's resistance to uniform compression and provides an indication of its hardness. Shear modulus measures a crystal's resistance to shear deformation and provides an indication of its rigidity. Young's modulus represents crystal's resistance to changes in length under tensile stress [3,4]. Poisson's ratio in crystals is significant as it describes the anisotropic elastic deformation, revealing how the crystal deforms in one direction when stressed in another direction and also it is key indicator of mechanical performance. The three dimensional variation of elastic moduli represents the stability of crystals, more the spatial variation of elastic moduli more will be the stability of crystal[5,6].Hexagonal crystals exhibit anisotropic behavior in their physical and mechanical properties, due to its unique symmetry and its dependence on the ratio vertical axis to horizontal axis. Due to high elastic constants, high birefringence and high negative dispersions, hexagonal crystals have their applications in hexagonal circular photonic crystal fibers and sensors in the field of communications[7].The number of independent elastic constants for a three dimensional crystal depends on symmetry of crystal system. For a general anisotropic crystal there are a maximum of 21 independent elastic constants, but for a hexagonal crystal its elasticity is specified by six different elastic stiffness constants C_{11},C_{12},C_{13},C_{33},C_{44} and C_{66}, only five of them are independent since $C_{66}=\frac{1}{2}(C_{11}-C_{12})$ [8].The Born criterion is a set of rules for determining the mechanical stability of crystalline solid. It states that a crystal is stable if it's internal energy increases for any small change in strain [9].Mathematically, for a hexagonal crystal necessary and sufficient conditions for stability of a crystal are,

$C_{11}>|C_{12}|$, $C_{44}>0$ and $(C_{11}+C_{12})C_{33}>2C_{13}^2$.

The stiffness matrix must be positive definite for the crystal to be mechanically stable, imposes specific inequalities on the combinations of elastic stiffness constants that depend on the crystal symmetry. The elastic stiffness constant matrix for a hexagonal crystal system, when represented in 6× 6Voigt notation, is a symmetric with five independent and one dependent non-zero elastic constants [10,11].The elastic stiffness matrix for hexagonal crystal is of the order 6× 6and denoted by C_{ij},

$$C_{ij}=\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{(c_{11}-c_{12})}{2} \end{bmatrix}$$

The eigenvalues of stiffness matrix in crystals are fundamentally related to crystal's mechanical stability, resistance to deformation along specific directions and modes of atomic vibration. A crystal is mechanically stable if and only if all eigenvalues of its elastic matrix are positive. If one or more eigenvalues are zero, it indicates lack of resistance to specific type of deformation. If eigenvalues are negative, it shows structural instability indicating that crystal could spontaneously deform into a new configuration associated with a phase transition [12].The velocity of primary and shear waves in a crystal depends on the materials elastic constants and its density-ρ. Due to anisotropy of crystal, wave velocity differ depending on the direction of wave propagation and polarization. The wave velocity has significance in materials characterization[13].The velocity of primary waves (V_p) and shear waves (V_s)in a crystal along c-axis are given by,

$$V_p=\sqrt{\frac{c_{33}}{\rho}} \qquad \text{and} \qquad V_s=\sqrt{\frac{c_{44}}{\rho}}$$

Oxides are the compounds with one or more oxygen atoms combined with another element. α-Al_2O_3 and ZnO are amphoteric oxides which reacts with both acids and bases. Oxides, based on their elastic constants used to manufacture ceramics, composites, protective coatings, solid oxide fuel cells, photonic ceramics and optoelectronic devices. Elastic constants of oxides are important in applications where mechanical properties are coupled with electrical, optical and acoustical performance [14,15]. Nitride is a compound in which nitrogen is bounded to less electronegative element. Nitrides with high elastic constants are used in high temperature lubricants, cutting devices, abrasives and hard coatings. β-Si_3N_4 is covalent nitride belongs to category of high performance advanced ceramics. It has high strength, hardness but low thermal expansion with high resistance for thermal shock. Hexagonal boron nitride, h-BN is a ceramic material with layered structured similar to graphite with high thermal conductivity. Due to its layered structure, it is slippery acting as good lubricant at high temperature [16]. Carbides are the compounds with carbon atom and one or more metallic or semi metallic elements. They are known for their exceptional hardness, brittleness and very high melting point. Carbides has an intensive applications in high temperature environments like furnace components and rockets [17]. Silicon carbide is a material consists of pure silicon and carbon.SiC-4H and SiC-6H are binary carbides with high elastic constants and elastic moduli, widely used in high power, high frequency and high temperature electronic devices due to its wide energy gap.SiC-4H wafers are suitable for a range of applications including power electronics, green energy generation and LEDs.SiC-6H is used in abrasives, UV Photodiodes, radiation hardened electronics for military and nuclear fields [18,19].

2. Materials and methods

The reported crystal structure data of α-Al_2O_3 [20], ZnO [21],β-Si_3N_4 [22], h-BN [23], SiC-4H [24] and SiC-6H [25] aregiven in the table 1, is used for computation. General Utility Lattice Program (GULP) is a freely available software wherein the input files needs crystal structure data and starting parameters for Buckingham potential. With the crystal structure data as input file with slight modification in the format, using Buckingham potential to GULP [26-28], we have computed physical parameters such as 6 elastic stiffness constants for sample hexagonal crystals, P-wave and S-shear wave velocities Using ELATE tensor analysis online program with elastic stiffness constants matrix of order 6×6as input file the physical parameters like elastic moduli, energy eigenvalues and 3D variation of elastic moduli are computed[29].

Table 1. Crystal structure data of sample crystals

	Category	Sample	Cell Parameters						Space Group	Ref
			α^o	β^o	γ^o	a in Å	b in Å	c in Å		
1	Oxides	α-Al_2O_3	90	90	120	4.758	4.758	12.992	$R\bar{3}c$	[20]
		ZnO	90	90	120	3.248	3.248	5.203	P63mc	[21]
2	Nitrides	β-Si_3N_4	90	90	120	7.607	7.607	2.911	$P6_3/m$	[22]
		h-BN	90	90	120	2.504	2.504	6.661	$P6_3/mmc$	[23]
3	Carbides	SiC-4H	90	90	120	3.079	3.079	10.082	$P6_3mc$	[24]
		SiC-6H	90	90	120	3.810	3.810	15.124	$P6_3mc$	[25]

3. Results and discussions

Elastic stiffness constants for sample crystals are computed and given in table 2. Further, the computed values are compared with the reported experimental values and in the same table. The units and descriptions of the symbols are given with details of the compounds at the bottom of the table.

Table 2. Computed elastic stiffness constants for sample crystals

		C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	Ref
1	Computed	504.2	163.9	128.1	502.4	156.9	170.0	
	Exptl	495	160	115	497	146	--	[30,31]
2	Computed	206	118.6	106.3	213.4	43.2	43.4	
	Exptl	209	120	104	218	44.1	--	[31,32]
3	Computed	439.2	198.7	130	582.9	103.5	120.3	
	Exptl	433	195	127	574	108	119.0	[30,33]
4	Computed	821.4	160.4	3.9	24.1	7.2	326.0	
	Exptl	811	169	0	27.7	7.7	--	[34,35]
5	Computed	509.2	107.2	50.2	551.2	153.6	201.1	
	Exptl	507	108	52	547	159	--	[34,36]
6	Computed	510.6	99.4	44.1	573.0	166.8	205.6	
	Exptl	502	95	--	565	169	203	[34,36]

1- α-Al_2O_3 ; 2- ZnO ; 3- β-Si_3N_4; 4- h-BN ; 5-SiC-4H ; 6- SiC-6H ; C_{ij} – in GPa

From table 2, it is clear that the computed values of elastic stiffness constants are in close agreement with reported experimental values. Elastic stiffness constant C_{11}=821.1GPa is maximum, for h-BN. It indicates that crystal h-BN is extremely stiff against small uniaxial strains applied in the plane along a-axis directions and crystal is much stiffer in plane than out of plane due to week bonding between inter layers along c-axis. A maximum value of C_{12}=198.7GPa is observed for β-Si_3N_4, indicating that to produce a small elastic strain along b-axis, a large stress is to be applied. It also shows a strong elastic anisotropy of crystal along b-axis. Higher value of C_{13}=130GPa for β-Si_3N_4 indicates its incompressibility under hydrostatic pressure and ensures high mechanical stability. Higher value of C_{33}=582.9GPa for β-Si_3N_4, indicates strong bonding along c-axis, driven by rod like arrangement of SiN_4tetrahedra in β-Si_3N_4 enhancing axial rigidity. It also indicates crystal has high elastic anisotropy which affects applications in high temperature ceramics where c-axis alignments boost fracture toughness and thermal shock resistance. A maximum value of C_{44}=166.8GPa is observed for SiC-6H, which shows crystal has strong resistance to shear deformation along c-axis. This higher value makes it exceptionally harder and suitable for high stress applications like cutting tools, bearings and power electronics under harsh conditions. Elevated value of C_{66}=326GPa is observed for h-BN. This higher value makes h-BN more appropriate for fracture toughness with suitability for 2D nano electromechanical systems, high temperature lubricants and insulators.

In crystals, P-waves and S-waves refer to primary and secondary phonon modes, which describe atomic vibrations in the lattice. Crystal anisotropy causes P-and S-wave velocities to vary directionally, deviating from isotropic predictions due to non-uniform elastic stiffness tensor components. P-wave and S-wave velocities in crystals are significant as they reveal the material's fundamental elastic properties, its anisotropy, composition and its internal structure including presence of micro cracks or fluids.

Table 3 shows the computed values of P- and S-wave velocities for sample crystals. The units and descriptions of the symbols are given with details of the compounds at the bottom of the table.

Table 3: Computed P- and S-wave velocities for sample crystals

Sample	V_p	V_s
1	11.23	6.28
2	6.16	2.77
3	13.52	5.69
4	3.38	1.85
5	13.36	6.92
6	13.40	7.22

1- α-Al_2O_3 ; 2- ZnO ; 3- β-Si_3N_4; 4- h-BN ; 5-SiC-4H ; 6- SiC-6H ;
V_p– P- wave velocity in Km/s, V_s– S- wave velocity in Km/s

A high P- wave velocity of 13.52 Km/s is observed in β-Si_3N_4 indicating high stiffness, high density with low porosity and few micro cracks in the corresponding crystal. A high S- wave velocity of 7.22 Km/s is observed in SiC-6H, indicating SiC-6H is more rigid, dense, well compacted and possess strong elastic properties.

Table 4 shows the computed elastic moduli and poison's ratio in Vioght, Reuss and Hill averaging schemes for sample crystals. The units and descriptions of the symbols are given with details of the compounds at the bottom of the table.

Table 4: Computed elastic moduli and poison's ratio

Sample	Averaging scheme	B	Y	S	σ
1	Vioght	261.22	418.02	169.47	0.2332
	Reuss	260.95	415.87	168.45	0.2343
	Hill	261.09	416.95	168.96	0.2338
2	Vioght	143.09	123.60	45.57	0.3560
	Reuss	143.07	122.68	45.20	0.3570
	Hill	143.08	123.14	45.38	0.3565
3	Vioght	264.3	340.14	132.30	0.2855
	Reuss	263.3	319.33	123.02	0.2978
	Hill	263.8	329.79	127.66	0.2916
4	Vioght	222.59	402.68	167.99	0.1984
	Reuss	23.29	36.41	14.68	0.2394
	Hill	122.94	219.63	91.34	0.2026
5	Vioght	220.58	447.34	192.49	0.1620
	Reuss	220.54	435.09	185.74	0.1712
	Hill	220.56	441.24	189.12	0.1665
6	Vioght	218.82	462.73	201.61	0.1475
	Reuss	218.54	452.72	195.95	0.1531
	Hill	218.82	457.74	198.78	0.1513

1- α-Al_2O_3; 2- ZnO; 3- β-Si_3N_4; 4- h-BN; 5-SiC-4H ; 6- SiC-6H;
B – bulk modulus in GPa; Y – Young's modulus in GPa; S – Shear modulus in GPa; σ – Poisson's ratio

All the sample crystals, except ZnO have significantly high bulk modulus. This shows excluding ZnO, the remaining crystals are highly resistant to compression with hardness and toughness nature. They are, therefore, suitable for applications like abrasives, cutting devices and useful in high pressure applications. Further, all the sample crystals have high young's modulus except ZnO. This high young's modulus make them suitable for their use in load bearing components, designing for micro and nano electromechanical systems. Higher young's modulus also indicates strong inter molecular or atomic bonding and highly ordered structure in these crystals. Except ZnO, all the sample crystals have significantly high shear modulus indicating high rigidity and hardness. The high value of shear modulus makes them to use in durable substrates in LEDs, in windows exposed to mechanical stress and in high pressure devices. Poisson's ratio of α-Al_2O_3,ZnO, β-Si_3N_4,and h-BN are in the range of 0.2 to 0.35, which shows these crystals are standard elastic solid, experiencing a proportional lateral contraction when stretched or expansion when compressed. Poisson's ratio around 0.15 to 0.17 is low in SiC-4H and SiC-6H, signifies crystals are highly stiff, relatively brittle and shows little tendency for lateral contraction compared to more ductile materials.

Figure 1 shows spatial variation of young's modulus in the samples.

Figure 1 : Spatial variation of young's modulus of the samples.

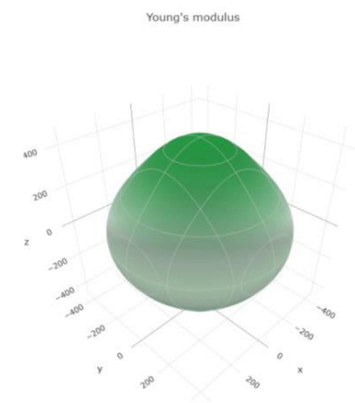


Figure 1.1

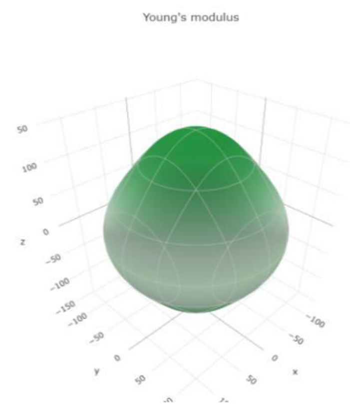


Figure 1.2

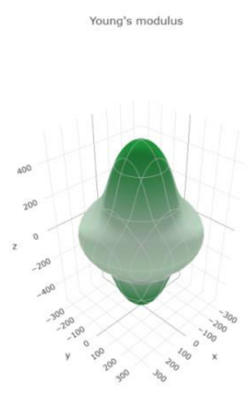


Figure 1.3

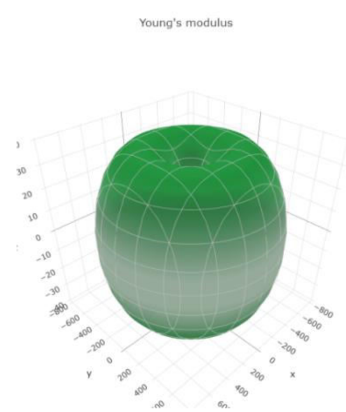


Figure 1.4

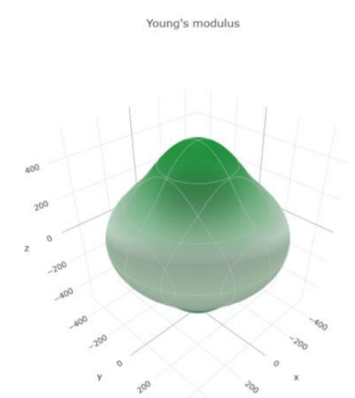


Figure 1.5

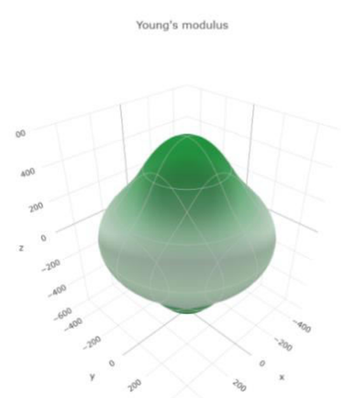


Figure 1.6

Fig-1.1, Fig- 1.2, Fig- 1.3, Fig -1.4, Fig -1.5 and Fig -1.6 represents Spatial variation of young's modulus in the samples1- α-Al_2O_3 ;2- ZnO ;3- β-Si_3N_4; 4- h-BN ; 5- SiC-4H and 6- SiC-6H respectively.

Figure 2: Shows spatial variation of linear compressibility in the samples

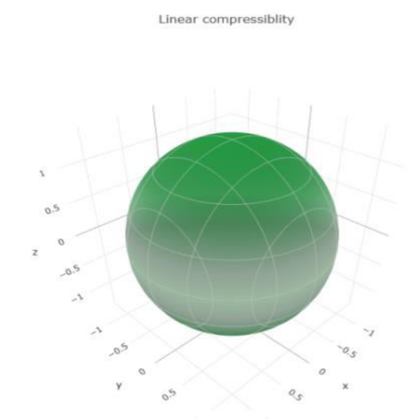


Figure 2.1

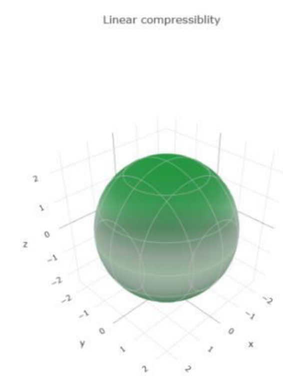


Figure 2.2

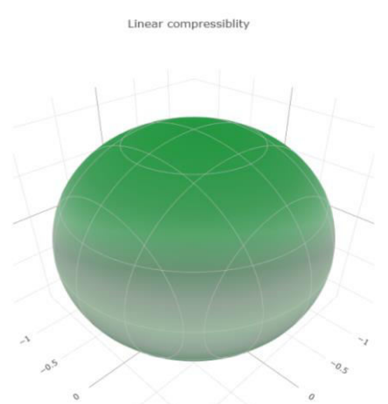
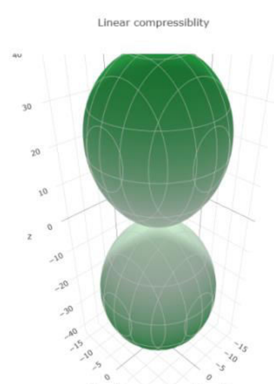


Figure 2.3



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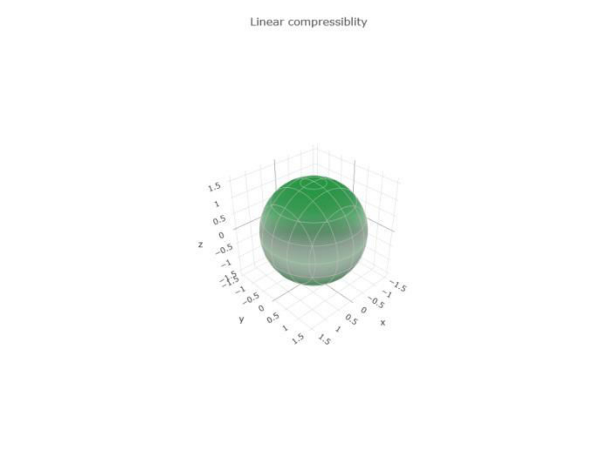

Figure 2.5

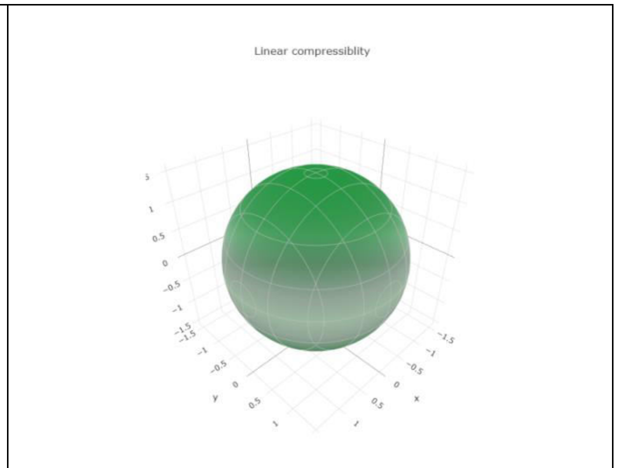

Figure 2.6

Fig-2.1, Fig- 2.2, Fig- 2.3, Fig - 2.4, Fig -2.5 and Fig -2.6 represents Spatial variation of linear compressibility in the samples1- α-Al_2O_3 ;2- ZnO ;3- β-Si_3N_4; 4- h-BN ; 5- SiC-4H and 6- SiC-6H respectively.

Figure 3: shows spatial variation of Shear modulus in the samples.

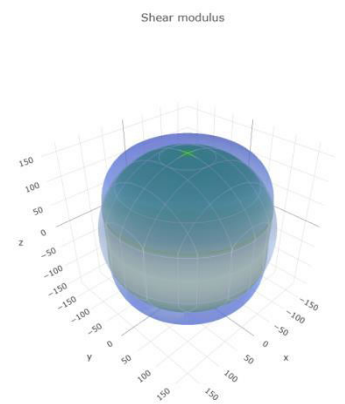

Figure 3.1

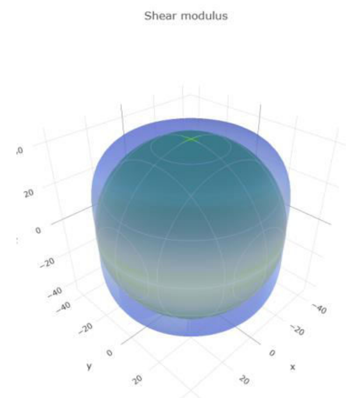

Figure 3.2

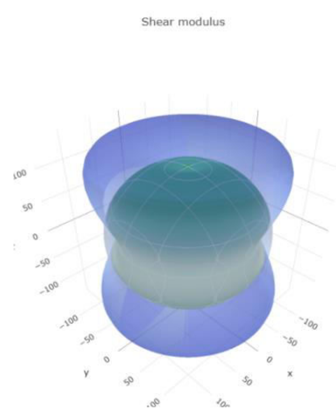

Figure 3.3

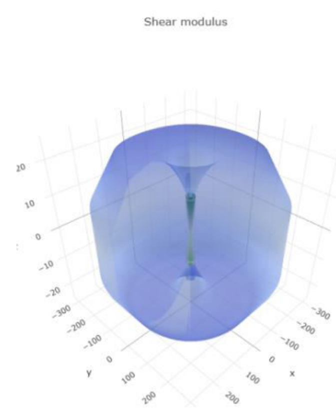

Figure 3.4

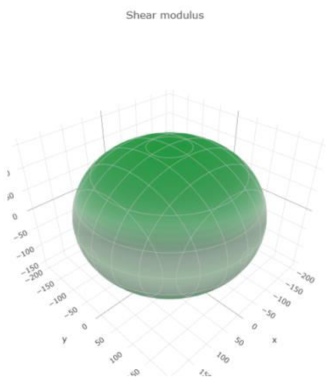

Figure 3.5

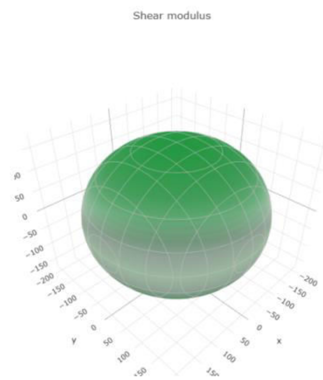

Fig-3.1, Fig- 3.2, Fig- 3.3, Fig-3.4, Fig-3.5 and Fig-3.6 represents Spatial variation of Shear modulusin samples1- α-Al_2O_3 ;2- ZnO ;3- β-Si_3N_4; 4- h-BN ; 5- SiC-4H and 6- SiC-6H respectively.

Figure 4: shows spatial variation of Poisson's ratio in the samples.

Figure 4: Spatial variation of Poisson's ratio in the samples.

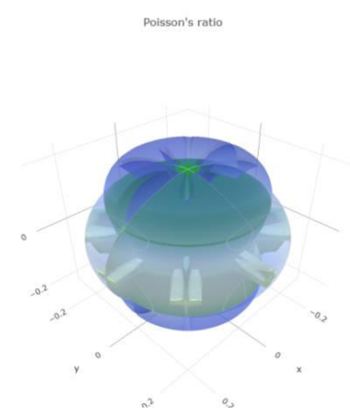

Figure 4.1

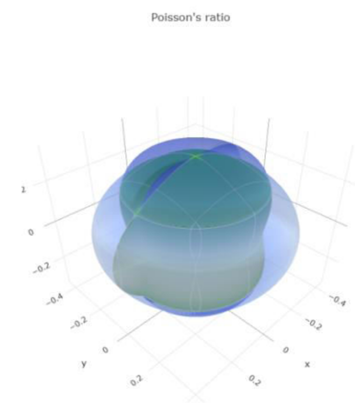

Figure 4.2

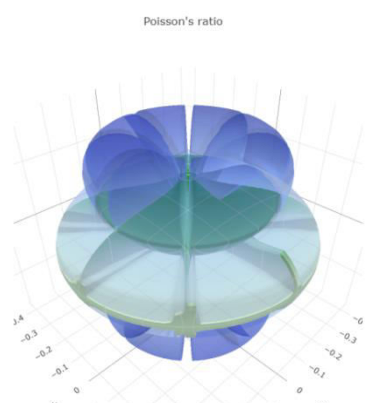

Figure 4.3

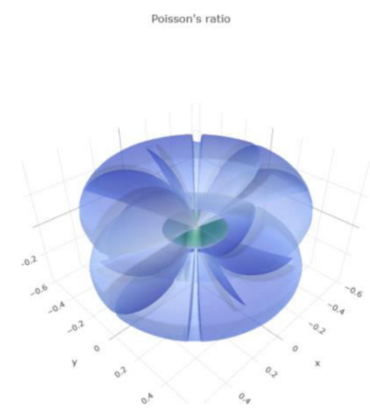

Figure 4.4

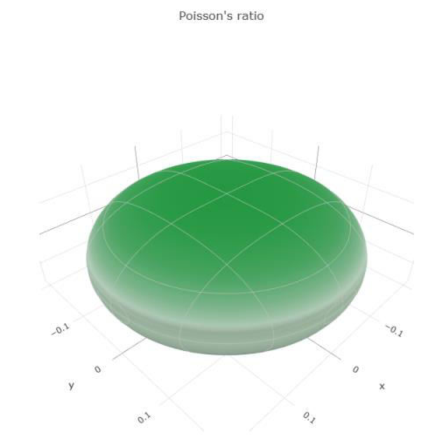

Figure 4.5

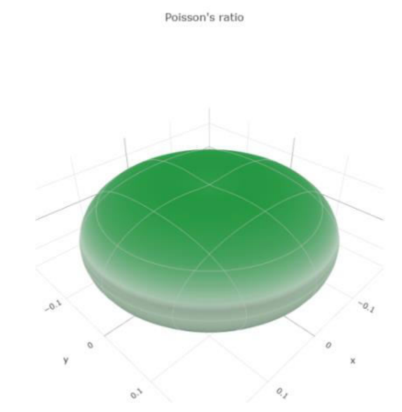

Figure 4.5

Fig-4.1, Fig- 4.2, Fig- 4.3, Fig-4.4, Fig-4.5 and Fig-4.6 represents Spatial variation of Poisson's ratioin the samples1- α-Al_2O_3 ;2- ZnO ;3- β-Si_3N_4; 4- h-BN ; 5- SiC-4H and 6- SiC-6H respectively.

Spatial variation of elastic moduli and Poisson's ratio represents the stability of crystal. From figures, it is clear that the spatial variation elastic moduli and Poisson's ratioof all the sample crystals are significantly high indicating that all the sample crystals are highly stable.

Anisotropy in elastic moduli and Poisson's ratio of the samples are computed and shown in table 5.Descriptions of the symbols are given with details of the compounds at the bottom of the table.

Table 5 ; Anisotropy in elastic moduli and Poisson's ratio of the samples

A	1	2	3	4	5	6
L	1.100	1.045	1.198	48.210	1.030	1.013
Y	1.138	1.219	1.854	39.150	1.377	1.359
S	1.191	1.186	1.726	45.900	1.547	1.475
σ	1.453	1.525	3.168	159.699	3.526	3.540

1- α-Al_2O_3 ; 2- ZnO ; 3- β-Si_3N_4; 4- h-BN ; 5-SiC-4H ; 6- SiC-6H ; A – Anisotropy in GPa ; L – Linear compressibility ; Y – Young's modulus in GPa ; S – Shear modulus in GPa ; σ – Poisson's ratio

From table 5, it is clear that anisotropy of elastic moduli and Poisson's ratio of h-BN is more compared to other sample crystals. It shows that elastic moduli vary significantly with direction. Further, this high directional dependence influences wave propagation and it can exhibit the most extreme mechanical behaviors.

The eigenvalues of the stiffness matrix for sample crystals is given in Table 6. The units and descriptions of the symbols are given with details of the compounds at the bottom of the table.

Table 6 : Eigenvalues of the stiffness matrix for sample crystals

Sample	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
1	156.9	156.9	170	340.3	386.04	784.46
2	43.2	43.2	43.4	87.4	108.72	429.28
3	103.5	103.5	120.3	240.5	424.51	796.29
4	7.2	7.2	24.06	326	661	981.83
5	153.6	153.6	201.1	402.2	505.74	662.06
6	166.8	166.8	205.6	411.2	526.45	656.55

1- α-Al_2O_3 ;2- ZnO ;3- β-Si_3N_4; 4- h-BN ; 5- SiC-4H: 6- SiC-6H

λ_i – eigenvalues of the stiffness matrix in GPa

It is evident from table 6 that, the eigenvalues of stiffness matrix λ_1,λ_2,λ_3,λ_4 and λ_5 are high for SiC-6H compared to that of other sample crystals. Interestingly, λ_6 is high for h-BN compared to that of other sample crystals. Higher value of λ_6 of h-BN compared to other samples indicates that, h-BN is adequately constrained and therefore stable and able to resist forces without undergoing infinite displacement.

4. Conclusions

The computed elastic stiffness constants of sample crystals are in close agreement with experimentally reported values. Elastic stiffness constant C_{11}=821.1GPa is maximum, for h-BN. It indicates that h-BN is extremely stiff against small uniaxial strains applied in the plane along a-axis directions. A maximum value of C_{12}=198.7GPa is observed for β-Si_3N_4, indicating that to produce a small elastic strain along b-axis, a large stress is to be applied. Higher value of C_{13}=130GPa for β-Si_3N_4 indicates its incompressibility under hydrostatic pressure and ensures high mechanical stability. Higher value of C_{33}=582.9GPa for β-Si_3N_4, indicates strong bonding along c-axis, driven by rod like arrangement of SiN_4tetrahedra in β-Si_3N_4 enhancing axial rigidity. A maximum value of C_{44}=166.8GPa is observed for SiC-6H, which shows crystal has strong resistance to shear deformation along c-axis. Elevated value of C_{66}=326GPa is observed for h-BN. This higher value makes h-BN more appropriate for fracture toughness with suitability for 2D nano electromechanical systems, high temperature lubricants and insulators. A high P- wave velocity of 13.52 Km/s is observed in β-Si_3N_4 indicating high stiffness, high density with low porosity and few micro cracks in the corresponding crystal. A high S- wave velocity of 7.22 Km/s is observed in SiC-6H, indicating SiC-6H is more rigid, dense, well compacted and possess strong elastic properties. All the sample crystals, except ZnO have significantly high bulk modulus. This indicates excluding ZnO, the remaining crystals are highly resistant to compression with hardness and toughness nature. Further, all the sample crystals have high young's modulus except ZnO, which make them suitable for their use in load bearing components, designing for micro and nano electromechanical systems. All the sample crystals excluding Zno, have significantly high shear modulus indicating high rigidity and hardness. Poisson's ratio of α-Al_2O_3,ZnO, β-Si_3N_4,and h-BN are in the range of 0.2 to 0.35, which shows these crystals are standard elastic solid, experiencing a proportional lateral contraction when stretched or expansion when compressed. Poisson's ratio around 0.15 to 0.17 is low in SiC-4H and SiC-6H, signifies crystals are highly stiff and relatively brittle. The spatial variation of elastic moduli of all the sample crystals are significantly high. anisotropy of elastic moduli and Poisson's ratio of h-BN is more compared to other sample crystals. It shows that elastic moduli vary significantly with direction. Further, this high directional dependence influences wave propagation and it can exhibit the most extreme mechanical behaviors. The eigenvalues of stiffness matrix λ_1, λ_2, λ_3, λ_4 and λ_5 are high for SiC-6H compared to that of other sample crystals. Interestingly, λ_6 is high for h-BN compared to that of other sample crystals. Higher value of λ_6 of h-BN compared to other samples indicates that, h-BN is adequately constrained and therefore stable and able to resist forces without undergoing infinite displacement.

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Suggestion for future work

- The study can be extended to derivatives of alkoxy-azoxybenzene liquid crystalline homologous series.
- The study can be extended to derivatives of azobenzene and azoxybenzene liquid crystalline compound and comparing the physical parameter with experimental results.
- Computation of elastic stiffness constants and elastic moduli of inorganic crystals and its comparison with experimental results, there by analyzing their applications can be carried out.
- Elecrtro-optical response simulations with respect to their elastic anisotropy can be studied.

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Competing interests

The authors declare no competing interests.