Mechanical stability parameters of chalcogenides and pnictides based optoelectronic materials

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A study of experimental data reveals that the bulk modulus of chalcogenides and pnictides based chalcopyrites ($A^{II}B^{IV}C_2^V$ and $A^IB^{III}C_2^{VI}$) can be explained by a simple scaling rule that rely only on the crystal ionicity, ionic charge product, and the melting temperature. PVV theory of crystal ionicity, temperature dependence of elasticity and product of ionic charge theory are taken into account for the study. Based on this result, a simple microhardness-bulk modulus relation is applied to evaluate the microhardness of the complex compounds; which correspond well with the experimental data and other published results. The proposed findings support in the modeling of emerging semiconductor materials and even understanding of their mechanical properties for optoelectronics, photovoltaic, electromagnetic (EM) screening, and spintronic applications.
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1. Introduction

Chalcogenides and pnictides based ternary tetrahedral ($A^{II}B^{IV}C_2^V$ and $A^IB^{III}C_2^{VI}$) semiconductors, which build a broader class of semiconducting materials with varied structural, mechanical, electrical, and optical properties and have attracted interest because of their growing scientific and technological applications. Among complex solids, ternary compounds are semiconductors having a large energy direct band gap, strong non linearity, low thermal conductivity, broad transparency window, lower melting temperatures, and a tetragonal chalcopyrite crystal structure [1-6]. Once studied for their low thermal conductivities, currently they are investigated for applications like as electromagnetic (EM) screening, spintronics [7-8], and photovoltaics [9]. One crucial area, chalcopyrites have wide applications is optoelctronics, such as laser diodes, optical parametric oscillators, nonlinear optical (NLO), Light emitting diodes and optical modulator devices [7-34]. They provide a great platform for generating electric fields in the visible, infrared, and terahertz (THz) spectral areas in nonlinear optics.

Large-area chalcopyrite crystal formation allows for the production of high-quality optical and optoelectronic materials and devices, particularly frequency converters for solid-state tunable

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laser systems [17-21].Furthermore, certain chalcopyrite crystals are projected to reveal a topological insulating phase in their natural state [22] and the potential for large amount of magnetic-impurity doping [7]. Structurally, these compounds are obtained from a source compound of structure II-VI and III-V correspondingly, for this purpose; group III element is replaced with a group II and group IV element or the group II by a group I and group III element, alternatively. Thus, tetrahedral bonding in these compounds drives from Zinc blende (ZB) geometry of the crystal [35, 36].Unlike, binary counterparts these posses great non linear susceptibility. Complex ternary materials are anisotropic due to the two different bonds in chalcopyrites. A high bifringence is produced by this anisotropy; which in turn conjugate with high nonlinear susceptibility makes ternary tetrahedral compounds very suitable for phase matching and structured second harmonic generation. In addition to these, additional significant industrial applications of ternary tetrahedral semiconductors are lasers, infrared oscillations, light-emitting diodes, infrared detectors, solar cells, superhard materials etc. [37-41]. In fact, current research on superhard materials makes the study of mechanical properties more appealing, because it is often assumed that harder materials, such as diamond, should have a higher elastic modulus [42, 43].

A large variety of solid-state properties have been described using an experimental model. Material scientists can declare crystal architecture, phase diagrams, lattice constants, and other allied properties, correctly. In recent past, a few concrete developments have been occurred in these and correlated areas [44-55]. These findings are based on significant innovations in empirical methods as well as, more critically, understanding gained from close collaboration between theorists and experimentalists exploring solid-state phenomena. In that case, empirical theories like plasmon energy, ionicity, electronegativity, empirical radii, and valence electron have become useful [44-52]. These theories are directly related to the electrical forces of the chemical bond and therefore render a way to understanding and categorizing various elemental characteristics of molecules and compounds. One of the most important requirements for modern materials whose products are employed in harsh environments is their ability to withstand high temperatures. This explains why researchers are interested in researching the temperature-dependent variations in these materials' properties. In recent past, Verma [56] has calculated bulk modulus and microhardness of ternary tetrahedral compounds with the help of outer shell electron and $k_B T_m/\Omega$ (T_m= melting temperature, Ω = atomic volume, k_B = Boltzmann's constant) normalization theories.

Here, we have presented an empirical method for bulk modulus determination of chalcogenides and pnictides based semiconductors based on the concept of valence electrons, ionicity, and different melting temperature of the compounds at ambient temperature and pressure; and also determined the microhardness by applying proposed formula. The obtained results are in accord with the results reported by previous researchers. As the experimental data of bulk modulus is available for only few compounds so, the proposed relation will prove of immense help of a large group of researchers to determine bulk modulus (B), microhardness (H) and other related properties.

2. Theoretical background

The bulk modulus determines materials resistance against shape deformation when undergoes compression. Anderson and Nafe [57] were first to put forward an analytical relation for bulk modulus in terms of specific volume $B_o \sim V_0^{-x}$ at sea-level pressure. But, this relation holds good for only specific group of compounds, here exponent 'x' varies with group of compounds. x=1 (for alkali halides, fluorides, sulfides, and telluride) and x=4 (oxides). Later on, various theorists have reported the values of B for numerous solid-state compounds [51, 53, 58-61]. For rocksalt structured compounds, Cohen [51] proposed the isothermal bulk modulus B at zero pressure as a function of bond length d (Å) as follows:

$$\text{for alkali halides B [GPa]} = 550/ d^3 \qquad (1)$$

$$\text{for zinc blende B [GPa]} = 176/ d^{3.5} \qquad (2)$$

In the semiconductors of group IV, III-V and II-VI,

$$B \text{ [GPa]} = (1971-220\lambda) \, d^{-3.5} \tag{3}$$

Here empirical parameter of crystal ionicity $(\lambda) = 0, 1, 2$ for IV, III-V, and II-VI compounds, respectively and d - bond length.

Lam et al. [62] have been developed an empirical relationship for bulk modulus to lattice parameters based on pseudopotential and local-density formalism as follow:

$$B = 1971 \, d^{-3.5} - 408 \, (\Delta Z)^2 \, d^{-4} \tag{4}$$

Here $\Delta Z = 2$ and 1 for II-VI and III-V group compounds.

Neumann [63] has analyzed the tendency in the bulk modulus of the elemental, binary, and ternary semiconductors of tetrahedral coordination and noticed that B is purely estimated by the volume of the unit cell and the spectroscopically established bond ionicity as follows:

$$B = b \, V^{-n} \tag{5}$$

$$b = b_o \, (1 - b_1 f_i) \tag{6}$$

Here V is the unit cell volume, b_o, b_1, and n are constants and f_i denotes crystal ionicity of the compounds.

Neumann [64] has also given another relation for bulk modulus in terms of melting temperature and microhardness of the compounds as;

$$B = c \, V_0^{-k} H / T_m \tag{7}$$

Here T_m is melting temperature, H-microhardness, c and k to be determined by comparison with experiment.

Garbato et al. [72] have suggested that the crystal ionicity is the average between bond ionicities of bonds A-C and B-C in ternary tetrahedral structure due to two cation-anion bonds.

Gallardo [65] has analyzed the bulk modulus of $A^I B^{III} C_2^{VI}$ chalcopyrites and proposed an amendment in Cohen's expression (7), and modified bulk modulus is shown as;

$$B = (1971-200\lambda) \, d^{-3.5} - |\chi_{AC} - \chi_{BC}|^{2.5} \tag{8}$$

Here d-bond length, χ_{AC}, χ_{BC} -electronic susceptibilities of the bonds and $\lambda = 0.72$.

D. Sharma et al. [66] have suggested an analytical relation for the determination B as the function of melting temperature and inter-atomic distance as;

$$B = T_m d^{-3.15} \tag{9}$$

Verma et al. [67] have expressed bulk modulus of ternary tetrahedral ($A^{II} B^{IV} C_2^{V}$ and $A^I B^{III} C_2^{VI}$) chalcopyrites in terms of the product $Z_1 Z_2 Z_3$ and bond length d as follows:

$$B = (Z_1 Z_2 Z_3)^S \, V \, d^{-5} \tag{10}$$

Here atoms A, B and C have charges Z_1, Z_2 and Z_2; S and V are empirical constants that rely on compound geometry with values 0.15 and 4056 respectively.

Frost and Ashby [77] have been shown that Young's modulus (Y) as a elastic property strongly depends upon melting temperature T_m of polycrystalline materials, with the following relation;

$$Y = \frac{100 \, k_B \, T_m}{\Omega} \tag{11}$$

Here, Ω-atomic volume and k_B - Boltzmann constant.

Verma [56] has also suggested a relationship for bulk modulus as the function of charge on valence electrons and $k_B T_m/\Omega$ normalization of chalcopyrite ($A^{II}B^{IV}C_2^V$ and $A^I B^{III} C_2^{VI}$) semiconductors as;

$$B = A + S \times \sqrt[4]{Z_1 Z_2 Z_3} \times \frac{k_B T_m}{\Omega} \tag{12}$$

Here A and S are constants obtained from regression analysis with values 9.0942 and 38.4705, respectively.

It has been obvious that physical parameters are crucial for device development, but none has presented significant results on bulk modulus and microhardness through different methodologies. As, these moduli are much melting temperature, crystal ionicity and ionic charge dependent. So, we made a fresh empirical effort to reach accurate results close to experimental values using melting temperature, crystal ionicity and ionic charge of compound.
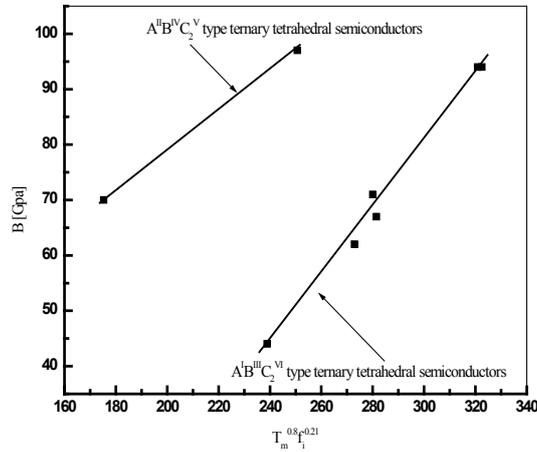
Fig. 1. Experimental B [GPa] versus crystal ionicity and melting temperature for ternary tetrahedral ($A^{II}B^{IV}C_2^V$ and $A^I B^{III}C_2^{VI}$) semiconductors. Bulk modulus of $A^I B^{III}C_2^{VI}$ lies on a line closely parallel to the line of the $A^{II}B^{IV}C_2^V$. Experimental data are drawn from [63, 69,70,71,72, and 73].
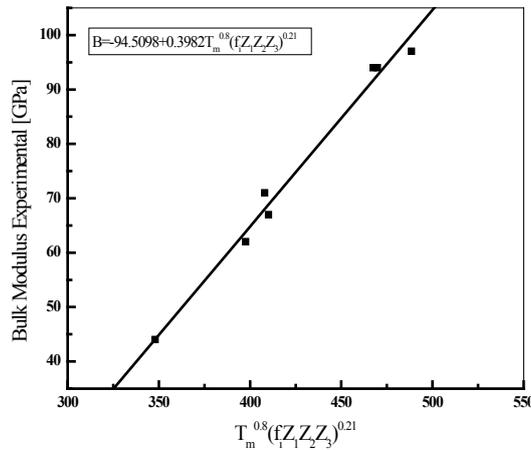
Fig. 2. Experimental B [GPa] for ternary tetrahedral semiconductors as a function of $T_m^{0.8}$ ($f_i Z_1 Z_2 Z_3)^{0.21}$. This straight line exhibits a linear relationship obtained by regression analysis of data. Experimental data are taken from [63].

So, considering the above empirical relations, applying the theory of ionic charge product given by Verma et al. [69] and using crystal ionicity and melting temperature of ternary tetrahedral semiconductors as input parameters, the experimental bulk modulus of these semiconductors shows linearity when graphed with respect to crystal ionicity and the melting temperature (K). The curves between experimental B [GPa] and $T_m^{0.8}f_i^{0.21}$ are shown in Fig. 1. It is obvious from the plot of experimental B and the product $T_m^{0.8}f_i^{0.21}$, the group $A^IB^{III}C_2^{VI}$ semiconductors lie along a line equidistant from the line to the group $A^{II}B^{IV}C_2^V$ semiconductors. This linearity originates from the ionic charges of the ternary tetrahedral semiconductors. When, we graphed existing experimental values of B with $Z_1\,Z_2\,Z_3$, melting temperature T_m and crystal ionicity f_i of ternary tetrahedral compounds at ambient temperature and pressure. A straight line is obtained for both the groups. It is shown in Fig. 2.

Bulk modulus has been demonstrated to have a rising tendency as $T_m^{0.8}f_i^{0.21}$ increases. Hence, on considering Eq. (12) we get the fact that B is a linearly proportional to the product of $T_m^{0.8}f_i^{0.21}$ and ionic charges. The obtained data from ternary semiconductors of tetragonal chalcopyrite geometry is plotted against $T_m^{0.8}f_i^{0.21}$ in figures 1 and 2. It is noteworthy that the method of determining bulk modulus by this mechanism creates a difference from experimental techniques, and this could develop errors.

Any mechanical change depends upon macro and micro variations of the compounds characteristics; so melting temperature represents this macro variation and crystal ionicity micro variation of the compound. As a result, a linear regression line is plotted for the bulk modulus, which results in an expression of bulk modulus [GPa] as;

$$B = P + Q \times T_m^{0.8}(f_iZ_1Z_2Z_3)^{0.21} \tag{13}$$

Here constants P and Q and regression coefficient R are presented in Table 1. Now, ionic charge product $(Z_1\,Z_2\,Z_3)$ is 48 for $A^{+2}B^{+4}C_2^{-3}$ (A= Cd, Zn; B= Ge, Si, Sn; C = As, P) and 12 for $A^{+1}B^{+3}C_2^{-2}$ (A = Ag, Cu; B = Ge, In, Al; C = As, P) valance structures. In table 1 probability parameter S shows the significance of regression as null i.e. there is no correlation.

Table 1. Ternary tetrahedral semiconductors data gives the following linear regression result.

Properties	P	Q	R	S
Bulk modulus	-94.5098±8.9417	0.3982±0.0208	0.9932	<0.0001

From Eq. (7), it is also clear that the microhardness of these compounds is linearly proportional to the bulk modulus and the same is proposed by Verma et al. [67] as;

$$H = K\,B^{K+1} \tag{14}$$

Here K is an empirical parameter and its value is 0.5 and 0.59 for ternary tetrahedral semiconductors, correspondingly.

3. Results and discussion

The modulus of elasticity values are significant data to reach a concrete conceptual understanding of material properties that are significantly related to the core electrons through valance electrons. The shift in the electronic charge centre towards the outer shell caused by variations in the wave function of outer electrons changes the mutual interaction between valence and core electrons. Consequently, the bond energy of the inner shell electrons changes and shifts the place of absorption edge. Valence electrons determine the ionic charge in a compound. Compound formation varies the ionic charge.. Since, bulk modulus B is the function of crystal ionicity f_i, which depends upon a fraction of ionic character due to symmetric and antisymmetric

portions of the potentials inside a unit cell. The change in the crystal geometry that occurs in a ternary tetrahedral compound, leads to the variation in crystal ionicity and therefore in the bulk modulus.

A detailed study on the correlation between transport characteristics and bond chemistry of the materials of distinct crystal structure was undertaken and found a relationship with the melting temperature of the compound. Tensile properties of the polycrystalline solids are related to melting temperature as a function of $k_B T_m / \Omega$ normalization. Considering these facts, we have evaluated bulk modulus and microhardness of ternary tetrahedral ($A^I B^{III} C_2^{VI}$ and $A^{II} B^{IV} C_2^V$) semiconductors. Experimental data for bulk modulus are handy for only some compounds in chalcopyrite series ($A^I B^{III} C_2^{VI}$ and $A^{II} B^{IV} C_2^V$) and theoretical data are reported for some compounds in the literature but these are mutually exclusive. A lot of efforts have been done to feed such leap in the study of mechanical properties of ternary tetrahedral semiconductors through analytical computations applying other's method, but in most cases values obtained vary significantly, and for various compounds, any satisfactory agreement hasn't been attained with available experimental data. Any examination of the effects of stress, strain, and pressure on the properties of compounds and thin epitaxial layers, on the other hand, demands the availability of precise elastic constant data. To obtain deep theoretical knowledge of material properties one should have availability of mechanical properties of material. In order to determine the mechanical properties; phonon-electron interaction processes intervene by deformation potentials, lattice anharmonicity effects and phonon density of states are prerequisite. The purpose of this study is to calculate and examine the now inadequate and conflicting data on compound's mechanical properties, as well as related experimental and theoretical data, that have been reported in the literature so far, in light of the importance of their knowledge and overall analysis of various types of material characteristics.

In this study, we have graphed the curve between bulk modulus versus melting temperature, crystal ionicity, and product of ionic charge in the compound and showed that bulk modulus can be evaluated from these parameters of the compounds. It is also shown that the bulk modulus of ternary tetrahedral compounds lies on a line closely parallel to each other according to their ionic charges and the results of calculations are presented in table 2.

The experimental results of microhardness (H) calculated by Garbato et al. [72] and Bodnar et al. [76] for comparison purposes are presented in table 3. The experimental values of microhardness of ternary tetrahedral compounds presented here have much variations as for CuAlSe$_2$ these are 210 and 325; for CuGaSe$_2$ these are 330,197,430 and 435; for CuGaTe$_2$ these are 215,180,360 and 347; for CuGaSe$_2$ these are 215,180,360 and 347; for CuInSe$_2$ these are 260,185 and 251; for CuInTe$_2$ these are 190,152 and 210; for AgGaS$_2$ these are 320 and 296; for AgGaSe$_2$ these are 230,143,450 and 310; for AgInSe$_2$ these are 127,230 and 187. These variations are mainly due to experiments being performed on the polycrystalline samples, because $A^I B^{III} C_2^{VI}$ compounds are anisotropic materials, changes in their composition from stoichiometry have a significant impact on microhardness measurements. The bulk modulus of ternary tetrahedral semiconductors has been calculated using the proposed relation (13) and values so achieved are put in relation (14) given by Verma et al. [67]. These values are presented in tables 2 and 3. The results of bulk modulus and microhardness estimated using these formulae are clearly more in agreement with experimental data than previous researcher's stated values. As an illustration, the results obtained for bulk modulus differ from experimental value of CuGaTe$_2$ by 0 %; of CuInSe$_2$ by 2.9%; of AgGaS$_2$ by 2.7%; of CdSiP$_2$ by 3.4%; of CuAlS$_2$ by 1.5%; of CuGaS$_2$ by 2.5% and of CuGaSe$_2$ by 4.3% in present study. Some higher deviations of elastic moduli of these ternary compounds are due to larger bond length. As the bond length increases heteropolar part of crystal ionicity also decreases and according to methodology used B and H also reduce, which widen the deviation of results. One more reason for large deviations of moduli values is lattice mismatch between substrate and deposited films. It is also noted that considered ternary compounds are more affected with temperature than ionicity as observed in calculated values.

Table 2. Calculated bulk modulus B [GPa] obtained through Eq. (13) for ternary tetrahedral semiconductors.

Solids	f_i [72,73]	T_m [K] [69,70,71]	B [63] Exp.	B [63,65]	B [67]	B [74]	B [56]	B [75]	B [68]	B This work
				Reported						
CuAlS$_2$	0.59	1570	94	94	94	94	93	95	93	92.61
CuAlSe$_2$	0.56	1273		69	74	69	68	73	73	61.98
CuAlTe$_2$	0.46	1163		45	52	45	53	42	53	45.18
CuGaS$_2$	0.60	1553	94	93	92	93	91	93	82	91.64
CuGaSe$_2$	0.56	1334	71	68	71	68	70	66	66	67.95
CuGaTe$_2$	0.47	1145	44	43	50	43	51	40	51	44.07
CuInS$_2$	0.64	1300		71	74	71	70	70	64	69.16
CuInSe$_2$	0.61	1263	62	54	59	54	61	52	63	63.82
CuInTe$_2$	0.53	1064		36	43	36	45	33	45	39.51
AgAlS$_2$	0.63	1420		73	74	73		70	73	80.56
AgAlSe$_2$	0.59	1223		55	59	55	59	52	59	58.72
AgAlTe$_2$	0.52	1002		36	43	36	43	33	43	32.71
AgGaS$_2$	0.61	1313	67	70	71	70	70	66	70	68.81
AgGaSe$_2$	0.59	1123		53	57	53	55	48	57	48.61
AgGaTe$_2$	0.51	1002		35	42	35	42	31	43	32.20
AgInS$_2$	0.68	1145		56	62	56	57	54	62	55.25
AgInSe$_2$	0.64	1053		42	49	42	47	38	50	43.77
AgInTe$_2$	0.57	965		28	36	28	38	25	37	31.34
ZnSiP$_2$	0.26	1523		120	110	120	121	117	114	111.20
ZnGeP$_2$	0.30	1298		108	101	108	99	105	104	92.03
ZnSnP$_2$	0.32	1203		84	82	84		82	83	83.42
ZnSiAs$_2$	0.18	1310		93	89	93	95	90	93	74.29
ZnGeAs$_2$	0.22	1148		86	84	86	81	83	85	63.91
ZnSnAs$_2$	0.33	1048		67	70	67	68	67	70	65.86
CdSiP$_2$	0.28	1393	97	97	91	97	102	92	97	100.03
CdGeP$_2$	0.32	1073		86	84	86	77	83	87	67.86
CdSnP$_2$	0.44	843		67	69	67	56	65	70	48.62
CdSiAs$_2$	0.19	1120		77	76	77	76	74	79	56.10
CdGeAs$_2$	0.23	938	70	70	70	70	62	67	72	41.53
CdSnAs$_2$	0.36	871		55	59	55	53	54	59	46.35

Table 3. Calculated microhardness H [all values in Kg/mm^2] by Eq. (14) for ternary tetrahedral semiconductors.

Solids	H [72,76] Exp.	H [72]	H [68]	H [67]	H This work
		Reported			
CuAlS$_2$	442	250, 261	251	456	445.59
CuAlSe$_2$	210,325	226,228	210	318	244.00
CuAlTe$_2$	182	255,210	166	188	151.83
CuGaS$_2$	430,445	230,245	229	141	438.63
CuGaSe$_2$	330,197,430,435	197,210	196	299	280.09
CuGaTe$_2$	215,180,360,347	240,185	161	177	146.28
CuInS$_2$	290,231	140	192	318	287.57
CuInSe$_2$	260,185,251	160,141	190	227	254.90
CuInTe$_2$	190,152,210	166,140	147	141	124.17
AgAlS$_2$		145	210	318	361.52
AgAlSe$_2$	160	176,135	179	227	224.96
AgAlTe$_2$	149	167,142	143	141	93.56
AgGaS$_2$	320,296	175,130	1048	299	285.41
AgGaSe$_2$	230,143,450,310	158,124	918	215	169.45
AgGaTe$_2$	135,180,260	166,142	673	136	91.34
AgInS$_2$	200	80	784	244	205.32
AgInSe$_2$	127,230,187	102,82	695	172	144.78
AgInTe$_2$	118,190	116,98	530	108	87.74
ZnSiP$_2$	1100	900	1048	1039	1057.17
ZnGeP$_2$	980	635	981	907	782.47
ZnSnP$_2$	650	530	673	651	669.33
ZnSiAs$_2$	920	820	784	742	556.70
ZnGeAs$_2$	680	630	695	677	438.23
ZnSnAs$_2$	455	430	530	507	459.69
CdSiP$_2$		730	834	769	893.43
CdGeP$_2$	565,410	470	725	677	482.09
CdSnP$_2$		255	531	495	283.73
CdSiAs$_2$		615	630	577	356.23
CdGeAs$_2$	470	470	553	507	220.84
CdSnAs$_2$	350,335	310	418	186	262.94

4. Summary and Conclusion

We can determine the mechanical properties of complex solids with the help of various approaches, yet owning to minute alteration in dimensions of a unit cell, the reliability of ascertaining these properties has always been a challenge to researchers. Besides, this has been revealed that mechanical properties like bulk modulus show a linearity relation once plotted against melting temperature and crystal ionicity; however they lie on distinct straight lines in accordance to the product of ionic charges of the atoms in compounds as shown in Fig.1. Hence, it

is clear from this discussion that the bulk modulus and microhardness describing the mechanical characteristics can be represented in terms of the product of melting temperature, crystal ionicity, and ionic charge product of the materials. This work found a very good agreement between the calculated values of the properties of the material and the values reported by previous researchers for the similar properties. It is also observed that the proposed formula is simple, widely applicable and thus results obtained are in better agreement with the experimental values than the values obtained through earlier empirical relations presented by previous researchers. The proposed formula will support material researchers in their quest for new semiconducting materials with the requisite mechanical properties for device applications in an analogous series of the materials.

Acknowledgements

References

[1] S. Tomar, R. Gautam, C.M.S. Negi, S.K. Gupta, S. R. Bhardwaj and A. S. Verma, Chalcogenide Letters, 16, 1 (2019).

[2] J. L. Shay and J.H. Wernick, Ternary Chalcopyrite Semi-conductors: Growth, Electronic Properties and Applications, Pergamon Press, Oxford, 11, 12 and 73 (1975); https://doi.org/10.1016/B978-0-08-017883-7.50012-3

[3] P. Singh, R. Gautam, S. Sharma, S. Kumari and A. S. Verma, Materials Science in Semiconductor Processing, 42, 288-302 (2016); https://doi.org/10.1016/j.mssp.2015.10.030

[4] P. Singh, S. Sharma, S. Kumari, Vibhav K. Saraswat, D. Sharma and A. S. Verma, Semiconductors, 51, 679 (2017); https://doi.org/10.1134/S1063782617050232

[5] J. D. Rowley, D.A. Bas, K. T. Zawilski, P.G. Schunemann, and A.D. Bristov, J. Opt. Soc. B 30, 2882 (2013); https://doi.org/10.1364/JOSAB.30.002882

[6] C. G. Ma and M. G. Brik, Solid State Communications 203, 67 (2015).

[7] Sheetal Sharma and A. S. Verma, European Physical Journal B, 87, 159 (2014); https://doi.org/10.1140/epjb/e2014-41097-2

[8] V. M. Novotortsev, A.V. Kochura, and S.F. Marenkin, Inorg. Mater. 46, 1421(2010); https://doi.org/10.1134/S0020168510130029

[9] Sheetal Sharma, A. S. Verma and V. K. Jindal, Materials Research Bulletin, 53, 218, (2014); https://doi.org/10.1016/j.materresbull.2014.02.021

[10] Y. X. Fan, R.C. Eckardt, R. L. Byer, R. K. Route, and R. S. Feigelson, Appl. Phys. Lett. 45, 313 (1984); https://doi.org/10.1063/1.95275

[11] S.C. Kumar, M. Jelinek, M. Baudisch, K. T. Zawiliski, P.G. Schunemann, V. Kubecek, J. Biegert, and M. Ebrahim-Zadeh, Opt. Expr. 20, 15703 (2012); https://doi.org/10.1364/OE.20.015703

[12] R. S. Feigelson and R. K. Route, Opt. Eng. 26, 113 (1987); https://doi.org/10.1117/12.7974036

[13] J.-B. Dherbecourt, A. Godard, M. Raybaut, J.-M. Melkonian, and M. Lefebvre, Opt. Lett., 35, 2197 (2010); https://doi.org/10.1364/OL.35.002197

[14] P.-H. Chuang, C. C. Lin, and R.-S. Liu, ACS Appl. Mater. Interfaces 6, 15379 (2014); https://doi.org/10.1021/am503889z

[15] M. C. Ohmer and R. Pandey, MRS Bulletin 23, 16 (1998); https://doi.org/10.1557/S0883769400029031

[16] V. Petrov, Physica status solidi c 14, 1600161 (2017); https://doi.org/10.1002/pssc.201600161

[17] H. P. Piyathilaka, R. Sooriyagoda, V. Dewasurendra, M. B. Johnson, K. T. Zawilski, P. G.

Schunemann, and A. D. Bristow, Optics Express 27, 16958 (2019); https://doi.org/10.1364/OE.27.016958

[18] B. N. Carnio, P. G. Schunemann, K. T. Zawilski, and A. Y. Elezzabi, Opt. Lett., 42, 3920 (2017); https://doi.org/10.1364/OL.42.003920

[19] J. D. Rowley, J. K. Wahlstrand, K. T. Zawilski, P. G. Schunemann, N. C. Giles, and A. D. Bristow, Opt. Express 20, 16968 (2012); https://doi.org/10.1364/OE.20.016968

[20] B. N. Carnio, K. T. Zawilski, P. G. Schunemann, and A. Y. Elezzabi, Applied Physics Letters 111, 221103 (2017); https://doi.org/10.1063/1.5006660

[21] B. N. Carnio, S. R. Greig, C. J. Firby, K. T. Zawilski, P. G. Schunemann, and A. Y. Elezzabi, Appl. Phys. Lett. 108, 261109 (2016); https://doi.org/10.1063/1.4955040

[22] W. Feng, D. Xiao, J. Ding, and Y. Yao, Phys Rev Lett 106, 016402 (2011).

[23] E. Bastola, K. P. Bhandari, I. Subedi et al., M. R. S. Comm. 8, 1 (1918).

[24] H. Sugimoto, H. Tomita, K. Yamaguchi, Y. Hirai, and T. Kato, Proc. PVSEC-29, 723 (2019).

[25] H. Nakamura, K. Yamaguchi, Y. Kimoto, Y. Yasaki, T. Kato, and H. Sugimoto, IEEE J. Photovolt.9, 1863 (2019); https://doi.org/10.1109/JPHOTOV.2019.2937218

[26] R. Woods -Robinson, Y. Han, H. Zhang, T. Ablekim, I. Khan, K. A. Persson, and A. Zakutayev, Chem. Rev. 120, 4007 (2020); https://doi.org/10.1021/acs.chemrev.9b00600

[27] T. Wada, Jpn. J. Appl. Phys. 60, 080101 (2021); https://doi.org/10.35848/1347-4065/ac08ac

[28] M.I. Alonso, K. Wakita, J. Pascual, and N. Yamamoto, Phys. Rev. B 63, 75203 (2001).

[29] M. Jing, J. Li, and K. Liu, IOP Conference Series: Earth and Environmental Science IOP Publication. 128,012087 (2018); https://doi.org/10.1088/1755-1315/128/1/012087

[30] Q. Lei, Z. Chunmei and C. Qiang, Sci. Technol. 16, 45 (2014).

[31] S. Sharma, A. S. Verma, R. Bhandari and V. K. Jindal, Comp. Mat. Sci. 86, 108 (2014); https://doi.org/10.1016/j.commatsci.2014.01.021

[32] A. H. Reshak and M. G. Brik, J. Alloys and Compounds 675, 355 (2016); https://doi.org/10.1016/j.jallcom.2016.03.104

[33] T. Dahame, M.A. Fadla, B. Bentria et al., Physica B: Cond. Matt. 561, 37 (2019); https://doi.org/10.1016/j.physb.2019.02.054

[34] Y.M. Basalaev, A.V. Kopytov, A.S. Poplavnoi et al., J. Struct. Chem. 58, 1588 (2017); https://doi.org/10.1134/S0022476617080169

[35] X. Jiang, W.R.L. Lambrecht, Phys. Rev. B 69, 035201 (2004).

[36] A.S.Verma and D. Sharma, Physica Scripta 76, 22 (2007); https://doi.org/10.1088/0031-8949/76/1/004

[37] M. Anani, C. Mathieu, S. Lebid, Y. Amar, Z. Chama, and H. Abid, Comp. Mater. Sci. 41, 570 (2008); https://doi.org/10.1016/j.commatsci.2007.05.023

[38] A.H. Reshak, Physica B 369, 243 (2005); https://doi.org/10.1016/j.physb.2005.08.038

[39] F. Chiker, B. Abbar, A. Tajder, S. Brsson, B. Khelifa, and C. Mathieu, Physica B 349, 181 (2004); https://doi.org/10.1016/j.physb.2004.03.087

[40] A. Chahed, O. Benhelal, H. Rozale, S. Laksari, and N. Abbouni, Phys. Stat. Solidi B 244, 629 (2007); https://doi.org/10.1002/pssb.200642050

[41] M. S. Yaseen, G. Murtaza, and R. M. A Khalil, Current Appl. Phys. 18, 1113 (2018); https://doi.org/10.1016/j.cap.2018.06.008

[42] C. G. Ma, D. X. Liu, T. P. Hu et al., Sc. Adv. Mater. 8, 446 (2016).

[43] N.M. Ravindran, D. Chen, Semiconductors: Other miscellaneous semiconductors and related binary, ternary, and quaternary compounds. Springer, 478 (2019).

[44] L. Pauling, The Nature of Chemical Bond. 3 Ed., Cornell University Press, Ithaca (1960).

[45] S. Sharma, A. S. Verma and V. K. Jindal, Mat. Res. Bull. 53, 218 (2014); https://doi.org/10.1016/j.materresbull.2014.02.021

[46] T. Lantri, S. Bentata, B. Bouadjemi, W. Benstaali, B. Bouhafs, A. Abbad and A. Zitouni, J. Magnetism and Magnetic Mat. 419, 74 (2016);

https://doi.org/10.1016/j.jmmm.2016.06.012

[47] V.Kumar and B.P.singh, Ind. J. Phys. 92, 29 (2018); https://doi.org/10.1007/s12648-017-1082-3

[48] S. Tomar, S.R. Bhardwaj, S.K. Gupta, and A.S. Verma, East Eur. J. Phys. 1, 47 (2020).

[49] Neeraj and A.S. Verma, East Eur. J. Phys. 1, 63 (2021).

[50] J.C. Phillips, Bonds and Bands in Semiconductors, Academic Press, New York (1973).

[51] M.L. Cohen, Phys. Rev. B 32, 7988 (1985); https://doi.org/10.1103/PhysRevB.32.7988

[52] V. Kumar and B.S.R. Sastry, J. Phys. Chem. Solids 66, 99 (2005); https://doi.org/10.1016/j.jpcs.2004.08.034

[53] Y. Al.-Douri, H. Abid, H. Aourag, Mater. Lett. 59, 2032 (2005); https://doi.org/10.1016/j.matlet.2005.02.011

[54] R. L. Moreira, A. Dias, J. Phys. Chem. Solids 68, 1617 (2007); https://doi.org/10.1016/j.jpcs.2007.03.050

[55] L. Q. Jiang, J.K.Guo, H.B. Liu, M.Zhu, X. Zhou, P.Wu, and C.H. Li, J. Phys. Chem. Solids 67, 1531 (2006); https://doi.org/10.1016/j.jpcs.2006.02.004

[56] A.S. Verma, Mat. Chem. Phy. 139, 256 (2013); https://doi.org/10.1016/j.matchemphys.2013.01.032

[57] O.L. Anderson, J.E. Nafe, J. Geophys. Res. 70, 3951 (1965); https://doi.org/10.1029/JZ070i016p03951

[58] S. K. Gorai, G. Parida, S.K. Sharma, RASAYAN J Chem., 10, 751 (2017).

[59] V. P. Gupta, S. K. Sipani, Phys. Stat. Solidi B 111, 295 (1982); https://doi.org/10.1002/pssb.2221110133

[60] A. Jayaraman, B. Batlogg, R.G. Maines, and H. Bach, Phys. Rev. B 26, 3347 (1982); https://doi.org/10.1103/PhysRevB.26.3347

[61] D. B. Srideshmukh and K.G. Subhadra, J. Appl. Phys. 59, 276 (1986); https://doi.org/10.1063/1.336826

[62] P.K. Lam, M.L. Cohen, and G. Martinez, Phys. Rev. B 35, 9190 (1987); https://doi.org/10.1103/PhysRevB.35.9190

[63] H. Neumann, Phys. Stat. Sol. a 96, K 121 (1986); https://doi.org/10.1002/pssa.2210960245

[64] H. Neumann, Cryst. Res. Technol., 23, 97 (1988); https://doi.org/10.1002/crat.2170230113

[65] P. G. Gallardo, Phys. Stat. Solidi b 182, K67 (1994); https://doi.org/10.1002/pssb.2221820234

[66] D. Sharma, A.K. Sharma, H. Singh, A. Kumar, Int. J. Sci. Res. Rev. 7, 547 (2019).

[67] A.S.Verma and S.R. Bhardwaj, J. Phys.: Cond. Matter 19, 026213 (2007); https://doi.org/10.1088/0953-8984/19/2/026213

[68] A.S. Verma and S.R. Bhardwaj, Phys. Stat. Sol. (b) 243, 4025 (2006); https://doi.org/10.1002/pssb.200642229

[69] V. Kumar and B.S.R. Sastry, J. Phys. Chem. Solids 63, 107 (2002); https://doi.org/10.1016/S0022-3697(01)00085-3

[70] M.S.Omar, Mater. Res. Bull. 42, 319 (2007); https://doi.org/10.1016/j.materresbull.2006.05.031

[71] V. Kumar, A.K.Shrivastava, Rajib Banerji, and D. Dhirhe, Solid Sate Comm. 149, 1008 (2009); https://doi.org/10.1016/j.ssc.2009.04.003

[72] L. Garbato and L. Rucci, Philo. Mag. 35, 1685 (1977); https://doi.org/10.1080/14786437708232990

[73] M.J. Bernard, Physique [Suppl.] 36, C3 (1975); https://doi.org/10.1051/jphyscol:1975301

[74] A.S. Verma, Phys. Status Solidi B 2, 345 (2009);

https://doi.org/10.1002/pssb.200844337

[75] A.S. Verma and S.R. Bhardwaj, Phys. Scr. 79, 015302 (2009);
https://doi.org/10.1088/0031-8949/79/01/015302

[76] I.V. Bodnar, B.V. Korzun and A.P. Chernyakova, Phys. Stat. Solidi a 101, 409 (1987);
https://doi.org/10.1002/pssa.2211010212

[77] A. G. Atkins, Deformation-mechanism maps (the plasticity and creep of metals and ceramics): by HJ Frost and MF Ashby, Pergamon, Oxford (1982).