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Full-potential investigations on the elastic and mechanical properties of the cubic biphasic forms of zinc sulphur through the methodology of Charpin

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ABSTRACT/RESUME

Abstract: *I apply the Full Potential Linearized Augmented Plane Wave FP-LAPW method based on the Density Functional Theory DFT within the most developed PBEsol2008 approximation together with the utilization of Gibbs programme to study the elastic, mechanical and electronic properties of ZnS into both cubic biphasic allotropic forms with low temperature structure i.e zinc-blende (B3) and high pressure structure which is rock-salt (B1) phase. Therefore, this study reports the results of the elastic constants and the mechanical quantities of this material and its dependences with temperature and pressure through the Charpin method. Furthermore, some quantities related to mechanical behaviours are well explained for these cubic phases. According to the theory of quantum field, the author finds that the sound velocities are evaluated in the classical mechanics. Moreover, the results show that Debye temperature is evaluated in the quantum mechanics and the Poisson's ratio (υ) is independent to the temperature. Cauchy's pressure and electronic charge density valid the covalent character of ZnS. I find great concordance between my results and the available theoretical and experimental data.*

I. Introduction

The small band gap semiconductors have application in the field of microelectronics [1]. The wide-gap semiconductor materials are very important for application in the fields of optical device technology et cetera. Among the wide band gap semiconductors Zn–VI group which have drew a great deal of attention in the last few years for their unique characteristics in different applications and so forth [2-12]. It is worth mentioning that there are several experimental methods to produce Zn–based semiconductor nanoparticles [13-20]. ZnS is the leading candidate due to its favourable physical properties especially in nanocrystalline form. It is astonishing that the elastic and mechanical properties of ZnS under high temperature and pressure are missing in literature. It is worthwhile to motion that the determination of elastic constants gives nexus with the mechanical and dynamical behaviours of materials, and provides an interesting definition about the nature of resultant forces in crystals. So, the elastic constants of anisotropic solids are very interesting physical quantities in the field of materials sciences. The coefficients of elasticity represent the interatomic potential and the anharmonicity of physical metallurgy. These quantities can describe a considerable source of informations on most metallurgical processes related to the interior of material such as: phase transition and precipitation. For the mechanic, the determination of the elasticity constants is essential for the design and calculation of the structures, as well as the confirmation of the theoretical models. Then, the estimation of these constants can be considered as an efficient and effective non-destructive means to determine the characteristics of the materials especially of their anisotropic damage [21]. Therefore, the acquaintance of elastic coefficients is prerequisite for various mechanical scope of application, such as: material response, strength, and so on. Some first-principles calculations have been focused on the elastic and mechanical properties of ZnS for different structures resulting from the temperature and pressure effects [22-29] . These crystallographic structures are well explained in the following references [30-33]. Generally, the technology of high pressure is widely used in the pharmaceutic compressed products. Also, this technology is more favourable than the high temperature in the sake to conserve the alkalization of liquid and colloidal products. To the best of my knowledge, neither measurements nor calculations of the temperature dependence of elastic and some mechanical properties structured ZnS have been reported before. Hence, the author study is the first attempt in this direction.

II. Calculation Method

All the present calculations are carried out with the Full Potential Linearized Augmented Plane Wave FP-LAPW implemented in WIEN2k_2013 code [34] together with the quasi- harmonic Debye model [35]. It is based on the framework of Density Functional Theory DFT [36-40] within the Generalized Gradient Approximation GGA in the new form PBEsol2008 proposed by Perdew et *al.* [41] which is an improved form of the most popular and physical Perdew-Burke-Ernzerhof (PBE) GGA [42] and which is also valid for all the compounds of chemical periodic table. Also, the use of Local Density Approximation LDA is correct, since the electronic structures of the compounds don't contain the orbital f. I expand the basis function up to $R_{MT}K_{MAX}$ = 8.5 (R_{MT} denotes the smallest atomic sphere radius and K_{MAX} gives the magnitude of the largest K vector in the plane wave expansion). The energy dividing the valence state from the core state was set as -6.0 Ry. The radii for the muffin-tin spheres were taken as large as possible without overlap between the spheres $R_{MT}^{S} = 1.8$ atomic units (a.u), $R_{MT}^{Zn} = 2.2$ atomic units (a.u). The maximum value for partial waves inside atomic spheres was l = 10 while the charge density was Fourier expanded up to G_{max} = 12 $(Ryd)^{1/2}$. Brillouin-Zone (BZ) integrations within self-consistency cycles were performed via a Monkhorst-pack method, using 10× 10 × 10 special k-point mesh for both (B3) and (B1) phases of ZnS. To obtain the elastic constants of ZnS with cubic structure, the author has used the numerical first-principle calculation by computing the compound of the stress tensor δ for small stains, using the method developed recently by Charpin [34]. In order to overcome the limitation of the standard potentials in the estimation of the electronic properties, good option is to use the newly approximation [43]. The recently developed modified Becke-Johnson (mBJ) functional [44] , is used to find the accurate electronic properties of electronic charge density, in excellent agreement with the experiments .

III. Results and discussions

III.1. Equilibrium lattice constants

I compute the lattice constants, bulk moduli and the pressure derivative of the bulk moduli by fitting the total energy versus volume. The calculated equilibrium lattice constants *a* for the (B3) and (B1) phases of ZnS are near similar to the values obtained through GGAPBE1996 and GGAWC2006 approximation in the author earlier studies [2, 45] and they are nicely compared to the experimental lattice parameters : *a*=5.413 Å [46] and *a*=5.06 Å [47] for the (B3) and (B1) phases of ZnS, respectively. This is caused by the use of GGA PBEsol2008 recent frame which is one of the families of GGA. GGA PBEsol2008 has been developed especially to enhance the description of exchange-correlation energy in materials, resulting in phases and energetic for densely packed solids and their surfaces which are closer to the experiment in most cases. On the other hand, it is worthy mention that the lattice parameters of materials can be measured by spectrometer X-Ray Diffraction XRD [48].

III.2. Elastic properties

III.2.1. Elastic stiffness constants at equilibrium conditions

Elastic constants of material are interesting because they are closely bound to several basic matter state phenomena. These quantities give information about the response of the material to the external applied forces. For the rhombohedron system ($3m, 32$ and $\bar{3}m$ classes), there are six elastic coefficients must be defined: C_{11}, C_{12}, C_{13}, C_{14}, C_{33} and C_{44}. Also, for the quadratic system ($4mm, \bar{4}2m, 422, 4/mmm$ classes) there are six elastic coefficients should be determined: C_{11}, C_{12}, C_{13}, C_{33}, C_{44} and C_{66}. On the other hand, for the hexagonal system (all the classes) five elastic constants could be estimated : C_{11}, C_{12}, C_{13}, C_{33} and C_{44} [49].

Due to the texture of the composite materials, its behaviours are strongly anisotropic. The measurement of elastic constants by conventional mechanical methods, such as, loading and extensometry requires a great large number of samples with suitable orientations. These destructive methods yield imprecise and incomplete results. Among the various methods of measuring the constants of elasticity developed to date, the non-destructive ultrasonic waves which considered as one of the best approaches in experimental solid mechanics [50].

So, the constants of material are interesting because they are closely bound to several basic matter state

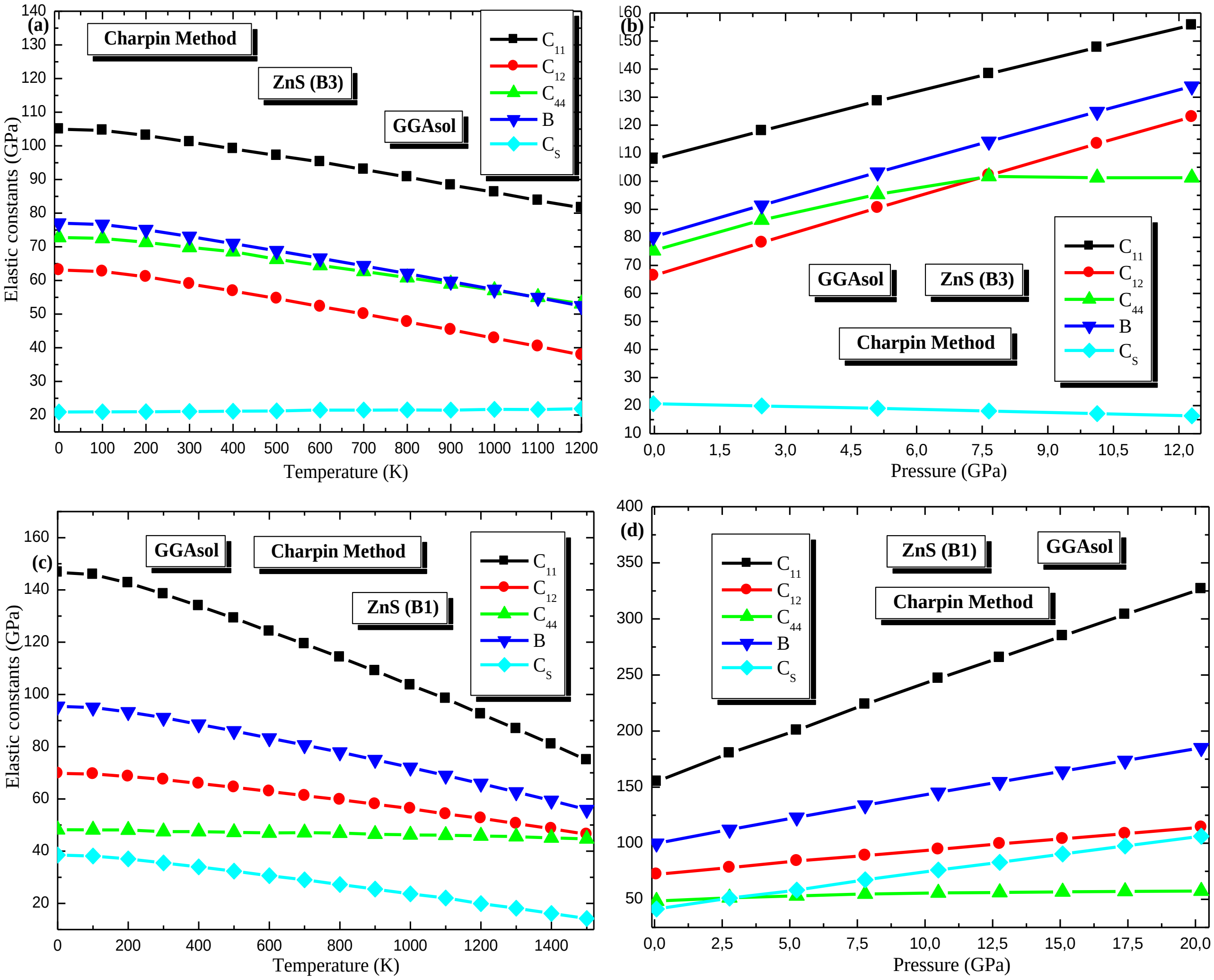

Figure 1. *Calculated temperature and pressure dependences of C_{ij}, C_s and bulk modulus B for both cubic phases of ZnS.*

phenomena. These quantities give information about the response of the material to the external applied forces. In this part, I am interested to investigate the elastic properties of the cubic phases. Hence, only three independent elastic coefficients, C_{11}, C_{12}, and C_{44}, needed to be calculated. Elastic constants C_{ij} are obtained using Charpin method implemented in WIEN2k code. Determination of C_{ij} values and the nature of strain must be defined. For the tetragonal strain conserving volume, I can induce C_{11} and C_{12} terms. To identify C_{44}, the author involves application of rhombohedral strain conserving volume. Further details of computational tools can be found in these references [51, 52].

The present values of the elastic constants for both cubic phases of ZnS are listed in Table 1 together with the available theoretical and experimental results. In view of this table, one can remark that the computed elastic constants (C_{11} and C_{12}) for (B1) phase are greater than those of (B3) structure. The traditional mechanical stability requires the conditions quoted in this reference[53]. The author results reveal that the cubic phases obey these stability criteria, showing that these phases are elastically stable. The calculated values of elastic constants for (B3) structure are in reasonable agreement with the previously reported results in Zinc-blende ZnS quoted in table 1. To date, no experimental data for elastic constants of (B1) ZnS are available to be compared with the author prediction.

III.2.2. The elastic properties of cubic phases of ZnS under temperature

Now, the author focuses this study to the temperature dependence of the single-crystals elastic constants C_{ij} and elastic moduli. The effect of the temperature and pressure on the elastic constants are taken into account using the quasi-harmonic Debye model [35].

The evolutions of the elastic constants, C_{11}, C_{12} and C_{44}, as function of temperature for the cubic phases are depicted in Fig. 1a and Fig. 1c. I note here that I am not aware of any experimental measurements or theoretical calculations on the temperature dependence of the elastic properties of ZnS in these cubic phases. In general, the elastic moduli of solid soften with increasing temperature due to the volume variation. From these Figs, C_{11} is commonly the largest in both value and slope. Interestingly, there are flips in magnitude between C_{44} and B when the (B3) phase is replaced by the (B1) phase. The majority of elastic constants decrease softly with increasing temperature. C_{44} and C_{12} are less sensitive to the temperature change compared to C_{11}. This behaviour of C_{44} and C_{12} versus temperature indicates that temperatures are not the most reason change of these structures to the shear deformation.

III.2.3. The elastic properties of cubic phases of ZnS under pressure

Now, the author is interested to study the elastic behaviour of the two allotropic forms of cubic ZnS under hydrostatic pressure effects. Variations of C_{11}, C_{12}, C_{44}, Cs and the bulk modulus B under pressure changes are given in Fig. 1b and Fig. 1d, respectively. A linear dependence in all curves, except for C_{44}, for both phases of ZnS is found. Whereas, for (B1) structure, I find quasilinear relationship between C_{44} and P. Even up to high pressures, the variation of C_{44} versus pressure is sublinear, for (B3) structure of ZnS.

III.3. Mechanical properties of ZnS

Accordingly, it is technically feasible to provide very important information about the mechanical and dynamic characteristics after the complete determination of the elastic properties. So, it is well known that the mechanical quantities can be measured by semi-empirical methods. The knowledge of mechanical properties is critical for ensuring reliable performance [54].

III.3.1. Shear modulus, sound velocities and Debye temperature

I define the shear modulus (G) as the measurement of the reversibility to the resistant deformation upon shear stress and it plays a dominant role in the prediction of hardness. It can be computed from the arithmetic average of the Voigt (G_V) and Reuss (G_R) [55-57] moduli. From table 1, the calculated (G) value of the (B1) phase is somewhat higher than that of the other phase under study. As a result, (B1) structure is stronger than the (B3) phase.

The longitudinal and transverse sound velocity can be defined via the shear modulus G and the bulk modulus B through Navier's equation [58]. Also, in the polycrystalline material, the average sound velocity is well determined in this reference [59].

The Debye temperature is a fundamental parameter for the physicists whereas the melting temperature is widely used in the fields of chemistry or physical metallurgy [60]. The Debye temperature may be determined from the average sound velocity V_m [61].

The relevant results for the mentioned above quantities along with the available theoretical and experimental results are presented in table 1. From this table, it is clearly seen that the author computed values correlate very well for both phases with the other calculated ones.

Based on the Theory of Quantum Field and according to the velocity of light C, I can distinguish two parts of mechanics [62]:

v ϵ] 0, 0.1×C[⇒ Classical Mechanics CM which is referred to us " Newtaonian Mechanics" after "Isaac Newton" and his laws of motion. Mechanics is subdivided into: statistics which models objects at rest, Kinematics which models objects in motion and dynamics which models objects subjected to forces. The CM of continuous and deformable objects is continuum mechanics, which can itself broken down into solid mechanics and fluid mechanics according to the state of matter been stated. The latter, the mechanics of liquids and gas include: hydrostatics, hydrodynamics pneumatics and aerodynamics and other field. CM can be used to describe many astronomical objects such as: galaxies, planets and certain macroscopic objects such as: organic molecules, theories such as fluid mechanics and kinetic theories of gas result from applying of CM in the microscopic systems.

v ϵ] 0.1×C, C [⇒ Relativistic or Einstein Mechanics

Based on results of sound velocities v presented in the precedent table 1 and the theory of quantum field, the author main very important ideas can be summarized as follows:

- Wien2k code contains the option of relativistic aspect and more informations are found in this reference [63]. So, the mechanics of Einstein is not used here and the sound velocities reported here are evaluated in the context of classical non relativistic mechanics because the quantities of sound velocities are situated in the range of v ϵ] 0, 0.1×C[where C is light velocity C= 2.99792458×10^{8} m/s. The CM produces very accurate results in the domain of every day experience. It is still very useful because it is still much simpler and easier to apply than other theories.
- The Planck's constant is specific character of quantum mechanics. Subsequently, Debye temperature is evaluated in the

context of quantum mechanics which confirms the validity of DFT theory because above this temperature, the thermal vibrations become more important than the quantum effects.

III.3.2. Kleinmann parameter, elastic anisotropy,Young modulus and Lame's coefficients

Kleinmann parameter (ζ) [64] is an important index which represents the relative position of the positive and negative ions lattices assembly[65].The well-known Kleinman parameter (ζ) for zincblende describes the relative positions of the cation and anion sublattices under volume by conserving strain distortions in which the positions are not fixed by symmetry [66]. It can be noted that the author values for ZnS are in excellent agreement with the theoretical data quoted in table 1. I recall that a low value of internal strain parameter implies that there is a large resistance against bond angle distortions while the reverse is true for a high value.

Elastic anisotropy (A) is another interesting factor that has an effective including in mechanical engineering field. It is interrelated with the possibility of producing micro cracks in the materials. For a completely isotropic system, A = 1. Deviation from unity evaluates the degree of anisotropy. To quantify the elastic anisotropy of the both phases, I have computed the anisotropy factor (A) from the present values of the elastic constants. From the computed anisotropy values in table 1, which also alike with the other theoretical data, one can see that (B3) phase is nearly isotropic, while (B1) structure show high amount of elastic anisotropy.

The polycrystalline Young's modulus (E) is then can be calculated from the mathematical equations reported in this reference [58]. From the present results of (E) listed in table 1, it can be stated that the (B1) phase is stiffer than the (B3) structure, since the Young's modulus (in GPa) is relatively very high for (B1) phase.

Correspondingly, Gabriel Lame's coefficients are the following: λ : called Lame's first parameter which does not have physical interpretation, but it serves to simplify the stiffness matrix in Hooke's law [67, 68]. μ : the Lame's second parameter or shear modulus (which referred to as G)).

The calculated Lame's coefficients in both structures of ZnS are given in table 1. Experimental and theoretical data on these coefficients for ZnS are not available for comparing with the author results.

III.3.3. Poisson ratio, Pugh's index (B/G) and Cauchy pressure

After the procurement of the necessary data, I now try to examine the ductile or brittle nature of the compound. I can describe the brittle/ductile characteristic of the crystals from some standard relations. Pugh's criterion [69] based on the ratio (B/G). If B/G is greater (lesser) than 1.75, the material behaves in a ductile (brittle) manner. Here, the value of Pugh's index (B/G) for (B3) phase is smaller than the critical value (1.75), meaning that the (B3) phase of ZnS is brittle in nature.

Afterwards, I would to elucidate the rule of Frantsevich et *al.* [70]. The distinction between ductility and brittleness of materials is possible via Poisson's ratio (υ) [58]. Applying this criterion, the critical value of material is 0.33. For ductile materials, the Poisson ratio is larger than 0.33, unless otherwise specified, the material appears in a brittle manner. The calculated and experimental values of (υ) are smaller than 1/3 for both structures. So, it is clear that both phases are placed in the brittle materials category.

Another index of the ductility and brittleness behaviours of the materials is the Cauchy's pressure (C_{12}-C_{44}). For the covalent bonding, (C_{12}-C_{44}) is negative and the material is brittle [71-73]. In other words, the zinc-blende ZnS is a brittle material with covalent character of bonding nature since the calculated value of Cauchy pressure is significantly more negative (-8.88).

III.3.4. Electronic charge density

To visualize the nature of the bound character and to explain the electronic charge transfer and the bonding properties of ZnS, I have explored to study the electronic charge density of ZnS. In view of the profile and contour plots of Fig. 2, one can note a symmetrical distribution of electronic charges with the majority lying between the atomic sites. This situation in the centre is similar from that found in semiconductors with diamond structure [74] where the electronic charge density is concentrated halfway between the two atoms. This curve indicates the presence of ionic bonding of the zincblende phase. Also, I observe the existing of covalent behaviour under lines gather Zn and S atoms. F. Benmakhlouf et *al.* [75] observed the presence of mixed–ionic–covalent bonding, with effective ionic charges close to $Zn^{+1}S^{-1}$ for the zinc-blende structure. On the other hand, A. Abbad et *al* .[76] confirmed in his investigation that ZnS has strongly covalent and partially ionic bond simultaneously. Absolutely, for all III–V and some II–VI binary semiconductors where the atoms are differents, the bound characters are partially covalent and partially ionic, with a strong covalent predominance [32]. Elsewhere, the covalent character of zincblende (B3) ZnS is confirmed in the section of mechanical properties.

III.3.5. The mechanical properties of zinc-blende ZnS under temperature

Table 1. *Calculated elastic constants and mechanical quantities (at P=0 GPa and T=0K): shear and Young moduli, Lame's coefficients, Kleinman parameter, Poisson ratio, B/G and anisotropy constant for (B1) and (B3) phases of ZnS. Also, computed longitudinal, transverse and average sound velocities and Debye temperatures concluded from mechanical parameters for both structures of ZnS: (B1) and (B3).*

	This study		**Literature Data**	
	(B1)	**(B3)**	**(B1)**	**(B3)**
C_{11} **(GPa)**	155.085	107.737	133.075 [a], 136.1[b]	96.283[a], 99.6 [b], 123.7 [c], 118 [d], 122 [e], 104.0[f] ,101±5 [g]
C_{12} **(GPa)**	72.3160	66.369	61.124 [a], 65.0 [b]	55.555[a], 57.0 [b], 62.1 [c], 72[d], 68 [e] 65.0 [f] ,64±5 [g]
C_{44} **(GPa)**	48.516	75.249	47.10 [a], 54.1 [b]	62.497[a], 50.5 [b], 59.7 [c], 75 [d], 57 [e] 46.2 [f] ,42±4 [g]
G (GPa)	45.525	45.018	42.3 [a]	40.590 [a], 31.2[h]
E (GPa)	118.567	113.758	108.8 [a]	102.1 [a], 105[i]
λ (GPa)	69.555	50.146		
μ (GPa)	45.525	45.018		
ζ	0.596	0.720	0.590 [a]	0.692 [a], 0.715 [d]
υ	0.297	0.263	0.287 [a]	0.257 [a], 0.32[h]
A	0.091	1.012	0.167 [a]	0.901 [a]
B/G	2.135	1.74		
V_T **(m/s)**	2988.036	3281.758		3300.00 [j] at (T=300K)
V_L **(m/s)**	5565.015	5756.615		5000.00 [j] at (T=300K)
V_m **(m/s)**	3309.540	3617.564		
Θ_D **(K)**	311.742	318.594		340 [j] at (T=0K)

[a]Ref.[22]Cal,[b]Ref.[25],[c]Ref.[29], [d]Ref.[28]Cal, [e]Ref.[27], [f]Ref.[77],[g]Ref.[78]Exp, [h]Ref [79] Exp, [i]Ref [80] from the bulk nanowires of ZnS, [d]Ref. Cal, [j]Ref [81] The sound velocities calculated along [100] propagation direction.

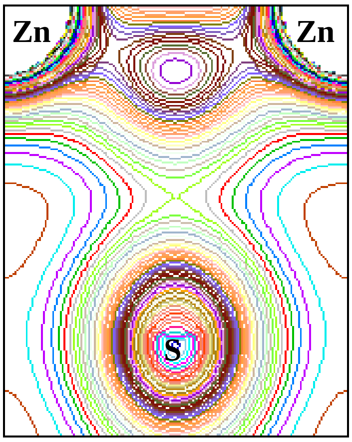

Figure 2. *Calculated electronic charge density of states for zinc-blende (B3) structure of ZnS using the modified Becke-Johnson approach.*

Until further notice, the dependence of mechanical properties of ZnS on temperature has not studied by theorists' physicists. In the subsequent text, I am the first who address this issue.

The temperature dependence of Kleinman parameter (ζ), Poisson ratio (υ) and anisotropy constant (A) has been calculated and illustrated in Fig .3a. As one can see from this graph, the mechanical indices (ζ) and (A) remain constant up to 100 K then show a decreasing trend with the increase in temperature. Moreover, I can also deduce that the Poisson ratio (υ) is nearly constant with increasing temperature. This is consistent well with other experimental study [82] concluding the independence of Poisson's ratio on the temperature.

The temperature effects on the Shear (G), Young Modulus (E) and Lame's coefficient (μ) are shown in Fig. 3c. From this figure, I can find that T < 100 K, the values of (G) ((G) is identical to (μ)) and (E) nearly keep constant for each quantity. When T > 100 K, all the quantities decrease significantly when the temperature increase. These results are close to the measurements as reported in this reference [82]. This latter found that the Shear (G) and Young Modulus (E) of cleartran multispectral zinc sulphur decrease with elevation temperature range from 289 K to 473 K.

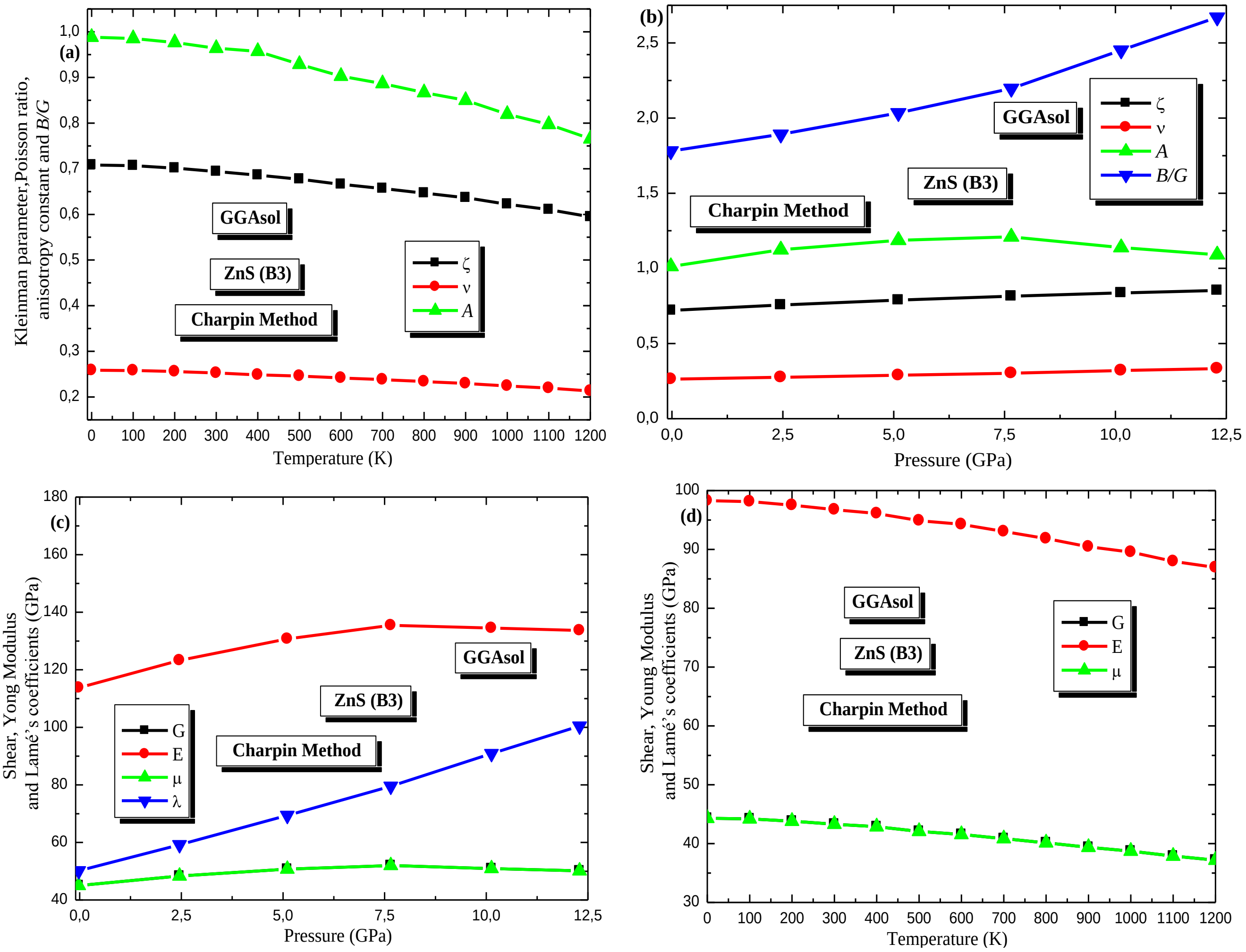

Figure 3. *Kleinman parameter, Poisson ratio, B/G ratio, anisotropy constant, shear modulus, Young modulus and Lame's coefficients as a function of: (temperature at P=0 GPa and pressure at T= 0 K) for zinc-blende (B3) ZnS.*

III.3.6. The mechanical properties of zinc-blende ZnS under pressure

The effects of the pressure on the above mechanical constants are shown in Fig. 3b. The pressure dependence of Kleinmann parameter (ζ) and Poisson ratio (υ) can be fit by a straight line but the changes of (B/G) index with hydrostatic pressure is quasilinear. It is beyond doubt that the elastic anisotropy (A) follows a nearly parabolic orbit variation with applied pressure.

Fig. 3d shows the evolution of the the Shear (G), Young Modulus (E) and Lame's coefficients (λ and μ) versus pressure. Lame's first parameter (λ) increases linearly with increasing pressure, as seen in the curvature. Furthmore, regarding the Young modulus values (E) and ((μ) = (G)), the general quasilinear dependence trend on the pressure is indicated.

IV. Conclusions

The GGAPBEsol within the framework of FPLAPW method together with Gibbs programme are successfully applied to investigate the elastic and mechanical properties of both allotropic cubic structures of ZnS. My main results can be summarized as follows:

- The calculated elastic stiffness coefficients appear that the cubic phases are elastically stable.
- The effects of temperature and pressure on the elastic constants are treated separately.
- The calculation and variations of mechanical properties of cubic ZnS within temperature and pressure, which have not yet calculated or measured, were obtained.
- It is observed that the Poisson ratio is almost constant versus the increment of temperature which is in accordance with the experimental variation.
- The results of Pugh's criterion and Cauchy's pressure show that the ZnS compound is brittle in nature with covalent bonding.
- Detailed comparisons are done with published experimental and theoretical data and show generally fairly agreement between them.

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