Original Research Article

Elastic Parameter & Properties of Ytterbium Chalcogenides (YbS, YbSe, and YbTe)

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Abstract

The present paper reports the numerical analysis of elastic parameters, such as shear constant, stiffness constant, Reuss shear modulus, Young's modulus, Poisson's ratio, and elastic anisotropy factor, of ytterbium chalcogenides. The theory has been developed to understand the mechanical phase transition phenomenon in ytterbium chalcogenides. The formulae are derived and used to obtain numerical values for different related parameters and the rock salt structure, which are useful for describing the phase transition event. The calculated values are in close agreement with the experimental results.

Keywords: Phase transition, Elastic parameter, Ytterbium chalcogenides

Introduction

Ytterbium (Yb) is a soft metallic element belonging to the rare-earth group, with the atomic number 70. Its compounds, generally represented as YbX (where X = S, Se, or Te), have attracted significant attention due to their complex structural and electronic characteristics. During phase transitions, changes in free energy are closely associated with modifications in the structural features of the phases, including both atomic and electronic configurations. The high-pressure phase transitions in alkaline-earth chalcogenides with rock-salt structures are fascinating, as they reveal the relationship between macroscopic and microscopic features of the system.

This study focuses on the elastic constants, as they provide insights into the structural, mechanical, and dynamical properties of solids. The elastic behavior and high-pressure phase transitions of ytterbium chalcogenides (YbX; X = S, Se, Te) are investigated using theoretical frameworks, including the Inter-Ionic Potential Model (IIPM). These compounds crystallize in the simple NaCl (rock-salt) structure and exhibit semiconducting behavior [1]. Interatomic potential-based models play a vital role in simulating B1–B2 structural transitions, while phenomenological models

have proven successful in analyzing phase transitions and structural characteristics across a variety of compounds.

Studies on ytterbium chalcogenides have demonstrated that phenomenological approaches effectively explain lattice dynamics, static and elastic properties, optical behavior, dielectric responses, and photo-elastic characteristics in semiconducting and ionic crystals. Moreover, research on the structural phase transition and superconductivity of lanthanide metals under high pressure has provided more profound insights into the fundamental physical mechanisms underlying lanthanide-based superconductivity. The comprehensive investigation of ytterbium chalcogenides underscores the importance of phenomenological models for accurately describing their structural and physical behavior under varying pressure conditions. These models effectively capture the intricate relationships between lattice dynamics, elastic properties, and electronic configurations, providing valuable insights into pressure-induced phase transitions. Moreover, studies on the structural phase transition and superconductivity of lanthanide Yb metal further deepen the understanding of the fundamental physical mechanisms governing lanthanide-based superconductors, highlighting the vital interplay between structural transformations and electronic properties in these complex systems [2,3]. Therefore, the present work is strongly motivated by the need to develop reliable theoretical models for ytterbium compounds, supported and validated by experimental data, to enhance the understanding of their high-pressure behaviors and physical properties.

The elastic properties of materials serve as a crucial indicator of their response to external stress and pressure, directly influencing the nature and dynamics of phase transitions under high-pressure conditions. Numerous studies have emphasized that the second-order elastic constants are key parameters for characterizing the mechanical stability and bonding strength of crystalline solids. Variations in these constants with pressure provide valuable information about the onset of structural instability leading to phase transitions. For ionic and semiconducting materials such as alkali and alkaline-earth chalcogenides, elastic properties have been extensively studied to elucidate the pressure-induced B1 (NaCl-type) to B2 (CsCl-type) structural transformations. Researchers such as Kanchana et al. [4] have demonstrated that elastic anomalies, including sudden changes in the bulk and shear moduli, serve as strong precursors of phase transitions. These behaviors are closely tied to the redistribution of electronic charge density and the modification of interatomic forces under compression, which collectively determine the stability and transformation pathway of the crystal structure.

In the context of rare-earth chalcogenides, including YbS, YbSe, and YbTe, the study of elastic constants under pressure has become increasingly important for understanding their unique electronic and structural properties. Ytterbium compounds are particularly intriguing due to the mixed-valence nature of Yb ions and the strong coupling between lattice and electronic degrees of freedom. Investigations using both experimental techniques, such as X-ray diffraction and ultrasonic measurements, and theoretical models, including inter-ionic potential and density functional theory (DFT) approaches, have revealed pressure-induced anomalies in their elastic behavior, indicating a transition from an ionic semiconducting phase to a metallic or mixed-valence phase. Furthermore, the correlation between elastic softening and electronic reconfiguration underscores the importance of elastic constants as a diagnostic tool in exploring high-pressure phase stability.

Hence, the systematic analysis of elastic properties not only aids in predicting phase boundaries but also contributes to a deeper understanding of the fundamental mechanisms governing structural phase transitions in Yb-based compounds.

Theoretical Methodology

Understanding the elastic constants of solids helps explain the relationships among structure, stability, and stiffness, as well as the mechanical and dynamical behaviors of crystals. The NaCl phase has been explained using the current model (IIPM), which has three model parameters. These parameters are used to calculate the second-order elastic constants using the following expressions.

$$C_{11} = (\frac{e^2}{4r^4})[-5.13Z(Z + 12f(r)) + A_1 + \frac{A_2 + B_2}{2} + 9.34Z\,(af'(r_0))] \quad (1)$$

$$C_{12} = (\frac{e^2}{4r^4})[0.24Z\,(Z + 12\,f(r)) - B_1 + \frac{A_2 - 5B_2}{4} + 9.34Z\,(af'(r_0))] \quad (2)$$

$$C_{44} = (\frac{e^2}{4r^4})[1.40Z\,(Z + 12\,f\,(r)) + \frac{A_2 - B_2}{4}] \quad (3)$$

where, $f(r)$ be the radial factor and $f'(r_0)$ derivative of $f(r)$, A_1 = longitudinal type lattice sum, A_2 mixed longitudinal–transverse projection, B_1 = first-derivative geometry sum, B_2 = cross-component first-derivative sum.

Knowledge of elastic constants is important for the stability of compounds, and many stability criteria are available. Followed the Born high-pressure stability criterion for an ionic crystal, according to which the stable phase of a crystal is one in which the shear elastic constant C_{44} is small and positive [5]. The IIPM is particularly well-suited for studying NaCl-type ionic solids because it accounts for long- and short-range forces and polarization corrections. Uses a small number of physically meaningful parameters and provides better agreement with experimental elastic data and pressure-induced behaviors.

Hence, compared to rigid or oversimplified models, the IIPM offers a balanced and physically realistic framework for explaining the elastic, structural, and dynamical properties of ionic crystals such as YbS, YbSe, and YbTe.

The elastic energy density must be a positive definite function of strain. To fulfill the above criterion, the principal minors (Eigen values) of the elastic constant matrix should all be positive. Thus, the stability of NaCl type structure in terms of elastic constants should satisfy the following conditions.

$$B_T = (C_{11} + 2C_{12})/3 > 0, C_{44} > 0 \text{ and } C_s = (C_{11} - C_{12})/2 > 0 \quad (4)$$

The bulk modulus can be derived from elastic constants. The hardness and strength of materials are related to their elastic modulus, such as Young's modulus (Y), Bulk modulus (B_T), and the shear modulus (G). In general, the larger the modulus, the harder the material is.

$$B_T = \frac{C_{11} + 2C_{12}}{3} \quad (5)$$

$$G_V = \frac{2C_S + 3C_{44}}{5} \quad (6)$$

$$G_R = 15\left(\frac{6}{C_S} + \frac{9}{C_{44}}\right) - 1 \quad (7)$$

The Voigt shear modulus (G_V) and Reuss shear modulus (G_R) are based on energy considerations. The Voigt and Reuss equations represent upper and lower limits of the true polycrystalline constants, and recommend that a practical estimate of the shear modulus is the arithmetic value of the extremes.

The study of the pressure dependence of the second–order elastic constants for Ytterbium compounds is also important. As this area is unexplored for Yb compounds, and no experimental or theoretical data on the pressure-dependence of elastic constants are available. Using model parameters (b, ρ, and f(r)), pressure derivatives of second order elastic constants have also been computed, whose expressions are as follows:

$$\frac{dB}{dp} = -(3\Omega) - 1[13.99Z(Z + 12f(r)) + C_1 - 3A_1 + C_2 - A_2 - 167.78Zaf'(r) + 41.96Za^2f''(r)] \quad (8)$$

$$\frac{dS}{dp} = -(2\Omega) - 1[23.69Z(Z + 12f(r)) + C_1 + \frac{C_2 + 6A_2 - 6B_2}{4} - 50.09Zaf'(r) + 13.99Za^2f''(r)] \quad (9)$$

$$\frac{dC_{44}}{dp} = -(\Omega) - 1[-11.39Z(Z + 12f(r)) + A_1 - 3B_1 + \frac{C_2 + 2A_2 - 10B_2}{4} + 44.68Zaf'(r)] \quad (10)$$

Where, $\Omega = -2.34\,Z\,(Z + 12f(r) + A_1 + A_2 + 21.98Zaf'(r))$

The values of A_i, B_i, and C_i have been evaluated based on knowledge of b, ρ, and the polarization effect [6].

Analysis of Phase Transition

The study of elastic constants and their combinations is important for understanding elastic properties. It also provides valuable information on the mechanical and dynamical properties, such as the interatomic potentials operating in solids. In particular, they provide information on the stability and stiffness of materials. We have computed the second-order elastic constants. The shear (C_S) and stiffness constant (C_L) of a cubic crystal (YbX in either NaCl (FCC) or CsCl (BCC)) are given by:

$$C_S = \frac{C_{11} - C_{12}}{2} \quad (11)$$

$$C_L = \frac{C_{11} + C_{12} + 2C_{44}}{2} \quad (12)$$

Elastic constants are given by:

$$\xi = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}} \quad (13)$$

This describes the relative positions of the cation and anion sublattices under volume-conserving strain distortions for which positions have not been fixed by symmetry. However, the physical meanings of the ξ depend on each other. Instead of a uniaxial strain, a pure shear strain is applied to the crystal. The symbol ξ represents a lattice relaxation parameter or internal strain parameter that describes how the relative positions of the cation and anion sub-lattices adjust under volume-conserving strain distortions. ξ measures the internal displacement between the two-interpenetrating sublattices (cation and anion) in a crystal when an external strain (usually shear or non-uniform strain) is applied. In crystals like NaCl-type or similar structures with two atoms per primitive cell, external strain does not uniquely determine the atomic positions. The relative shift between the two atoms is characterized by ξ. It quantifies the degree of internal relaxation necessary to minimize the total energy (both bond-stretching and bond-bending contributions) under strain. The total energy is a sum of the bond-stretching and bond-bending terms. The ξ is derived in terms of the crystal's elastic parameters, C_{11} and C_{12} [7-10].

First, we have calculated the different elastic constants (C_{11}, C_{12} and C_{44}) based on Table 1.

Table 1 Different present data of elastic constant (GPa) for ytterbium chalcogenides

Compounds	Lattice constant (Å)	C_{11}	C_{12}	C_{44}
YbS	5.68	179.23	20.49	50.57
YbSe	5.93	159.50	13.09	50.18
YbTe	5.36	105.25	17.25	34.01

(Source: Verma, 2009)

Taking the values of C_{11}, C_{12} and C_{44} from Table 1, then calculate the shear constant and Stiffness constant for the compounds YbS, YbSe, and YbTe, and derive the bulk modulus from the elastic constants. According to Voight shear modulus G_V and Reuss shear modulus G_R which are energy considerations for YbS, YbSe, and YbTe. In this modulus, represent the upper and lower limits, and recommend a shear modulus for a cubic system.

$$G = \frac{G_V + G_R}{2} \quad (14)$$

Young's modulus is defined as the ratio of stress to strain, which is vital to understand the properties of solids. It is used to provide a measure of the solid's stiffness. The present values of Young's modulus increase from Te to S.

$$Y = C_{11} - \frac{2(C_{12})^2}{C_{11} + C_{12}} \quad (15)$$

Poisson's ratio of a material is a reflection of stress waves, which is important to know the hardness of compounds. I have calculated the Poisson ratio (σ) as:

$$\sigma = \frac{C_{12}}{C_{11} + C_{12}} \quad (16)$$

Poisson's ratio has two limits: it must be greater than -1 and less than or equal to 0.5. The elastic anisotropy factor (A) of a cubic crystal is defined as:

$$A = \frac{2C_{44} + C_{12}}{C_{11}} - 1 \quad (17)$$

The calculated anisotropy parameter of Yb compounds. For an isotropic crystal, the value of A is 1. Any value smaller or larger than 1 indicates the presence of anisotropy. The Cauchy relation $C_{12} - C_{44}$ = 2P (P; pressure) is valid only when all interatomic forces are central under static lattice conditions. At zero pressure, our calculations give negative values of $C_{12} - C_{44}$, showing violation of the Cauchy relation. Using the data from Table 1, the shear and stiffness constants using Equations (11) and (12) are determined. The shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor are shown in Equations (14), (15), (16), and (17). Numerical calculation values are given in Table 2.

Table 2 Calculated values of shear constant, stiffness constant, shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor

Compounds	C_S	C_L	ξ	G	Y	σ	A
YbS	79.37	250.29	0.26	92.7	175.026	0.102	-0.44
YbSe	75	136.47	0.23	89.23	175.52	0.075	-0.289
YbTe	44	95.26	0.31	56.756	100.39	0.14	-0.19

The calculated values (Table 2) and experimental values (Table 3) are compared with shear constant, stiffness constant, shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor, which are as follows.

Table 3 Experimental values of Shear constant, Stiffness constant, shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor

Compounds	C_S	C_L	G	Y	σ	A
YbS	79.37	147.77	59.67	147.17	0.1	-0.34
YbSe	73.20	134.92	58.96	156.94	0.07	-0.29
YbTe	44.00	94.08	37.31	100.08	0.14	-0.20

The variations of shear constant, stiffness constant, shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor with lattice constant of ytterbium chalcogenides are shown in Figures 1-6.

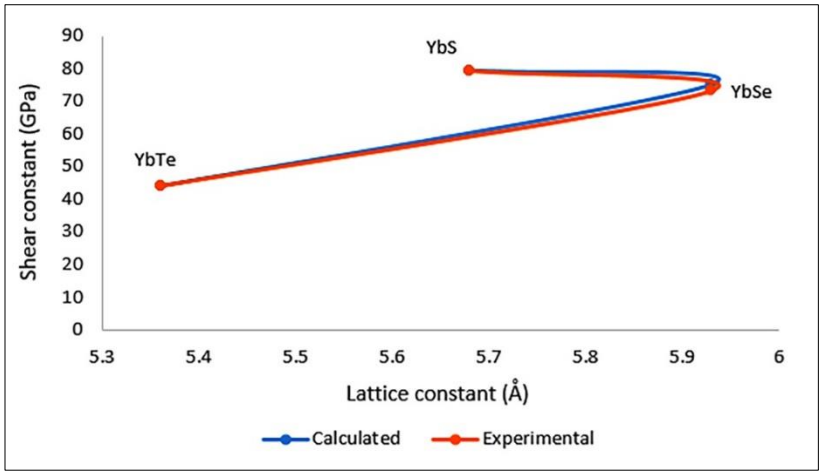


Figure 1 Variation of shear constant with lattice constant

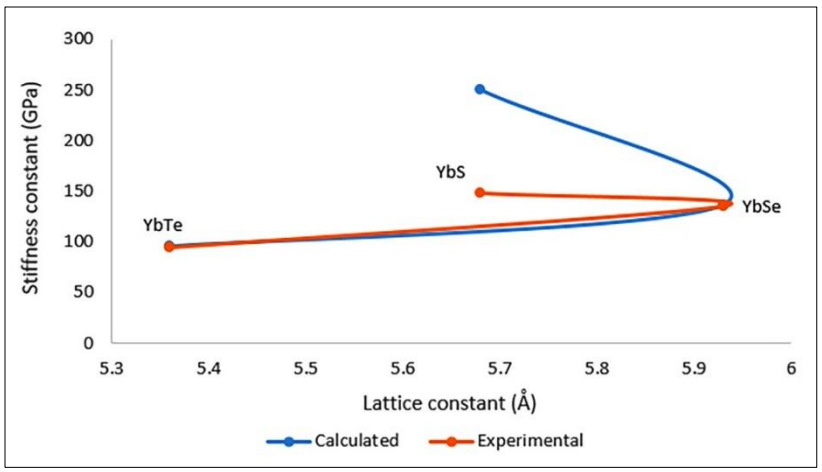


Figure 2 Variation of stiffness constant with lattice constant

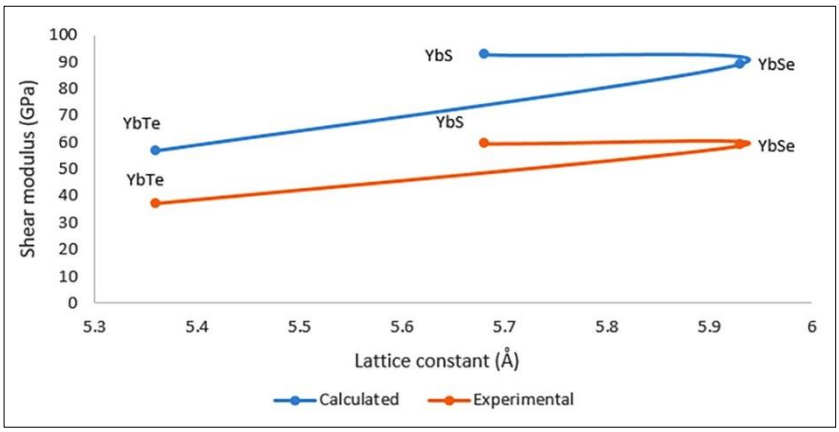


Figure 3 Variation of shear modulus with lattice constant

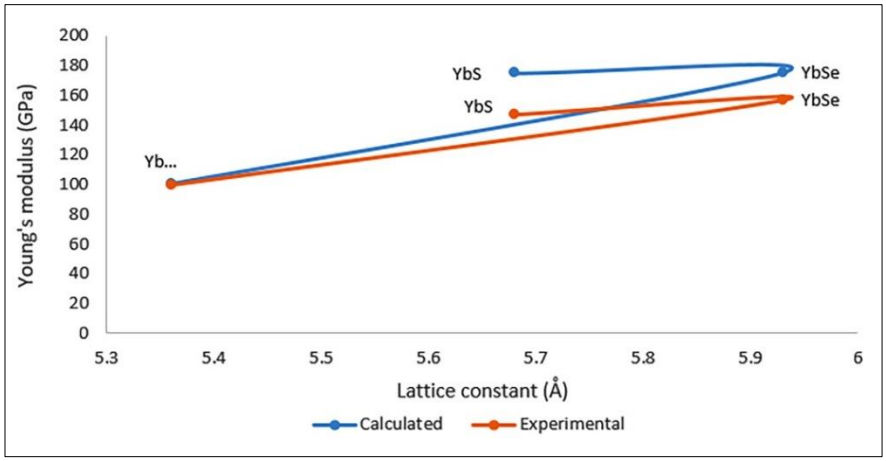


Figure 4 Variation of Young's modulus with lattice constant

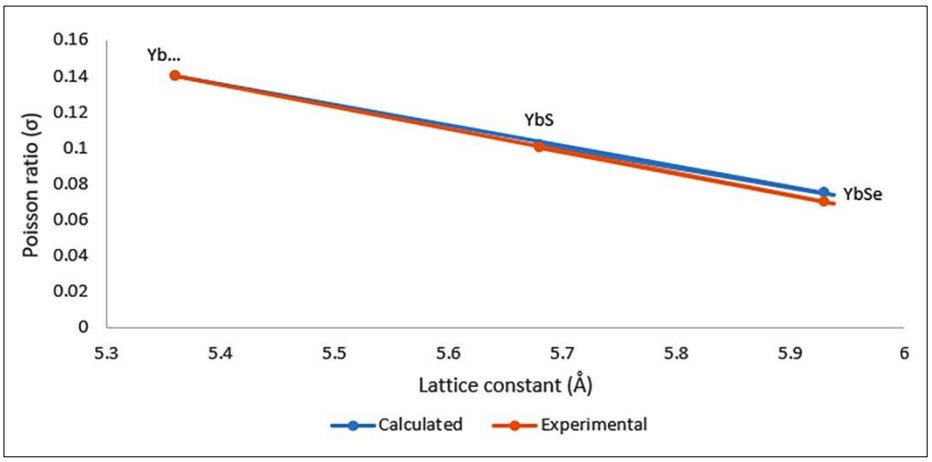


Figure 5 Variation of Poisson ratio with lattice constant

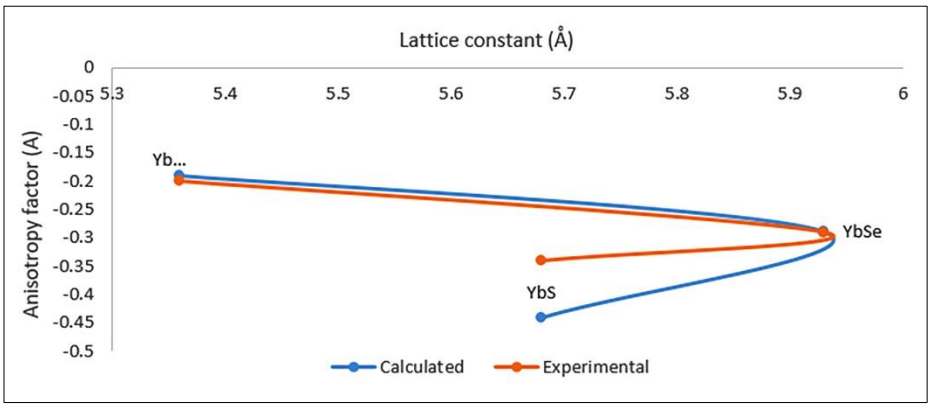


Figure 6 Variation of the Anisotropy factor (A) with lattice constant

The anisotropy parameter (A) and the parameter ξ are both important indicators of the elastic behavior and bonding nature in crystalline materials. The parameter ξ, which ranges from −½ to 1, describes the relative contribution of bond stretching and bond bending to the elastic energy of a crystal. Specifically, ξ = −½ corresponds to a condition where bond stretching requires no energy (indicating purely central forces), while ξ = 1 signifies that bond bending requires no energy (indicating purely non-central or angular forces). The anisotropy parameter A, on the other hand, reflects the degree of elastic anisotropy in a crystal and is given by A. For an isotropic material, A = 1; any deviation from unity (either smaller or larger) indicates anisotropy in the elastic response. The calculated A values for YbS, YbSe, and YbTe—0.44, 0.289, and 0.19, respectively—suggest a strong elastic anisotropy and predominantly central-force character in their bonding. These variations in A and ξ values highlight the differing strengths of interatomic interactions and angular rigidity among the Yb chalcogenides under study. According to Figure 1, the shear constant decreases with increasing lattice constant, indicating that larger atomic spacing weakens the material's resistance to shear deformation. In Figure 2, the stiffness constant decreases as the lattice constant increases, indicating that stretched atomic bonds lead to lower mechanical rigidity. Figure 3 predicted that the shear modulus decreases with increasing lattice constant, reflecting weaker atomic interactions and reduced elastic strength. Figure 4 shows that Young's modulus decreases with increasing lattice constant due to weakened interatomic forces and reduced structural stiffness. Poisson's ratio increases with lattice constant, suggesting that materials with larger atomic spacing exhibit greater lateral deformation under stress, as shown in Figure 5. In Figure 6. the decreasing anisotropy factor (A) values indicate increasing elastic anisotropy among Yb compounds, influenced by bond strength variations and lattice distortions.

Discussion

In the present study, the high-pressure phase transition and elastic properties of YbS, YbSe, and YbTe have been comprehensively analyzed. These compounds crystallize in the rock-salt (B1) structure at ambient conditions and exhibit ionic semiconducting behavior governed by the hybridized electronic states of ytterbium. The Yb atom, with an outer configuration of $4f^{14}5d^{0}6s^{2}$, interacts with chalcogen anions (S, Se, Te) through strong ionic and covalent bonding contributions. The

calculated elastic constants provide insights into the mechanical stability of these systems and reveal how lattice spacing influences their bonding strength and rigidity.

The results show that the shear and stiffness constants, as well as the shear modulus and Young's modulus, decrease with increasing lattice constant, indicating weaker interatomic bonding and lower resistance to deformation at larger atomic spacing. Conversely, smaller lattice constants correspond to stronger Yb–X interactions and higher stiffness. Poisson's ratio rises with lattice expansion. At the same time, the anisotropy factor and internal parameter (ξ) demonstrate significant elastic anisotropy across the YbX series, primarily due to variations in bond strength and lattice distortion. These observations confirm that mechanical strength is strongly correlated with crystal volume and bonding nature in Yb-based chalcogenides.

Under compression, these compounds undergo a pressure-induced structural transformation from the rock-salt (B1) to the CsCl-type (B2) structure. This phase change involves increased coordination and denser atomic packing, making the B2 phase energetically favorable at high pressure. The calculated transition pressures align closely with experimental findings, and minor deviations can be attributed to theoretical simplifications, experimental uncertainties, or lattice imperfections. The study confirms that the observed transitions are driven by both elastic deformation and electronic rearrangement, thereby validating the reliability of the adopted computational model.

The electronic structure plays a crucial role in governing these transformations. Under high pressure, the 5d conduction band of Yb broadens and shifts downward, overlapping with the localized 4f band, leading to a 4f–5d electronic transition and a gradual shift from Yb^{2+} to Yb^{3+} states. This hybridization enhances co valency and leads to a metallic character in the high-pressure phase. The coupling of elastic and electronic effects explains the volume collapse and changes in bonding nature during the transition. Overall, these findings provide significant implications for materials science, suggesting that Yb chalcogenides—with their tunable elastic and electronic properties—can serve in high-pressure sensors, thermoelectric devices, and nanoscale technologies, where controlled mechanical and electronic responses are critical.

Figure 1 depicts the relationship between the shear constant and the lattice constant. The shear constant reflects a material's resistance to shear deformation. As the lattice constant increases, the shear constant may show an increasing, decreasing, or non-linear trend depending on the atomic interactions. Variations in the lattice constant alter the interatomic spacing, which directly affects the forces binding the atoms. For instance, increasing the lattice constant might weaken these interactions, thereby lowering the shear constant. Conversely, a smaller lattice constant might indicate stronger bonding forces, resulting in a higher shear constant.

Figure 2 shows how the stiffness constant varies with the lattice constant. The stiffness constant is a measure of the material's ability to resist deformation under applied forces. Similar to the shear constant, the stiffness constant may either increase or decrease as the lattice constant changes. Changes in the lattice constant influence the mechanical rigidity of the crystal structure. Larger lattice constants often lead to reduced stiffness because atomic bonds are stretched, weakening their resistance to deformation. Conversely, smaller lattice constants typically result in higher stiffness due to stronger atomic bonds.

Figure 3 predicted that the shear modulus represents the material's ability to resist shear deformation and is derived from the shear and stiffness constants. The shear modulus often mirrors the trends observed in the shear constant and stiffness constant. As the lattice constant increases, the shear modulus might decrease due to weakened atomic interactions. The shear modulus depends on both the material's elasticity and its atomic structure. When the lattice constant increases, the atomic spacing grows, reducing the material's ability to sustain shear stress. Conversely, smaller lattice constants strengthen the atomic bonds, increasing the shear modulus. The variation of mechanical properties with lattice constant provides insights into the material's structural stability and mechanical behavior. These trends are critical in applications where materials are subjected to stress or deformation, such as in construction, aerospace, or nanotechnology. Understanding these dependencies also helps in material design, especially in tailoring properties for specific applications.

Figure 4 depicts the Young's modulus, which measures a material's ability to withstand uniaxial stress without permanent deformation. The graph likely shows how Young's modulus varies as the lattice constant changes. Generally, Young's modulus decreases with increasing lattice constant due to the weakening of interatomic forces as atoms are spaced farther apart. A smaller lattice constant results in stronger atomic interactions, which increase the material's stiffness. Conversely, a larger lattice constant reduces these interactions, leading to a lower Young's modulus. This behavior highlights the dependency of elastic properties on atomic structure.

Figure 5 shows that the Poisson ratio describes the ratio of transverse strain to axial strain when a material is stretched. The variation in Poisson's ratio with lattice constant may exhibit a trend depending on the material's atomic configuration and bonding characteristics. As the lattice constant increases, the degree to which a material contracts transversely under axial tension might change. Materials with strong atomic bonding (smaller lattice constants) often exhibit lower Poisson ratios, while those with weaker bonds (larger lattice constants) may have higher Poisson ratios. These trends help elucidate the balance between bond-stretching and bond-bending mechanisms.

Figure 6 predicted that the anisotropy factor indicates the directional dependence of mechanical properties. The calculated anisotropy factor values for the Yb compounds are 0.44, 0.289, and 0.19, which suggest significant anisotropy in their elastic properties. The parameter ξ describes the relative contributions of bond stretching and bond bending to the material's elastic response. For the given Yb compounds with A = 0.44, 0.289, A = 0.44, 0.289, A = 0.44, 0.289, and 0.19, 0.19, 0.19, the values suggest increasing anisotropy, likely caused by variations in bond strengths or lattice distortions. Anisotropy directly impacts the mechanical behavior, as the material exhibits different stiffness in different crystallographic directions. An interaction potential with significant overlap repulsion, valid only for the nearest-neighbor ions, was formulated to analyze the phase transition of ytterbium chalcogenides. The phase transition pressure is obtained using shear constant, stiffness constant, bulk modulus, shear modulus, Young's modulus, Poisson ratio, and anisotropy factor for YbS, YbSe, and YbTe. All calculated values are in close agreement with the available experimental values.

Conclusion

Recent theoretical approaches for predicting. The pressure-dependent phase transition shows that Ytterbium chalcogenides undergo a transition from a divalent semiconducting state to a trivalent metallic state. The elastic constants induced shear constant, stiffness constant, bulk modulus, shear modulus, Young's modulus, Poisson's ratio, and anisotropy factor versus lattice parameter are predicted. The calculated parameters for the ytterbium chalcogenides are in good agreement with the experimental results.

The main limitation of this method is that its predictive ability is limited to the explicitly considered surface structures, and there is always the risk of lower energy states. The variations of Young's modulus and Poisson's ratio with lattice constant demonstrate how atomic-level changes influence bulk mechanical properties. The range of ξ illustrates the fundamental trade-off between bond stretching and bending mechanisms in determining material rigidity and deformation behavior. The calculated anisotropy factors highlight directional differences in the mechanical properties of Yb compounds, which are critical for applications requiring specific directional strengths or stiffness. Additional mechanical properties, including shear modulus (G), Young's modulus (Y), Poisson's ratio (σ), and anisotropy factor (A), were derived. Calculations using the Voigt-Reuss-Hill approach provided practical estimates for these moduli.

The study also explored the relationship between elastic properties and lattice constants, revealing trends in stiffness and stability across YbS, YbSe, and YbTe. Experimental and theoretical values of the elastic parameters were compared, showing strong agreement. The anisotropy factor, which indicates the degree of elastic isotropy, was calculated, with values deviating from unity, suggesting anisotropic behavior.

References

[1] P. Strange, A. Svane, W. M. Temmerman, Z. Szotek and H. Winter, "Understanding the valency of rare earths from first-principles theory", Nature, 399, 756–758 (1999). https://doi.org/10.1038/21595.

[2] Q. Duan, J. Shen, Z. Zhong, H. Lu, and C. Lu, "Structural phase transition and superconductivity of ytterbium under high pressure", Physical Review B, 105, 214503 (2022). https://doi.org/10.1103/PhysRevB.105.214503.

[3] E. O. Gomes, A. F. Gouveia, L. Gracia, Á. Lobato, J. M. Recio and J. Andrés, "A chemical-pressure-induced phase transition controlled by lone electron pair activity", The Journal of Physical Chemistry Letters, 13, 9883–9888 (2022). https://doi.org/10.1021/acs.jpclett.2c02582.

[4] V. Kanchana, G. Vaitheeswaran, A. Svane, "Calculated structural, elastic and electronic properties of $SrCl_2$", Journal of Alloys and Compounds, 455, 480-484 (2008). https://doi.org/10.1016/j.jallcom.2007.01.163.

[5] T. Jaroń, J. Ying, M. Tkacz, A. Grzelak, V. B. Prakapenka, V. V. Struzhkin and W. Grochala, "Synthesis, structure, and electric conductivity of higher hydrides of ytterbium at high pressure", Inorganic Chemistry, 61, 8694–8702 (2022). https://doi.org/10.1021/acs.inorgchem.2c00405.

[6] P. Bharadwaj and S. Singh, "Pressure induced structural phase transitions—A review", Central European Journal of Chemistry, 10, 1391–1422 (2012). https://doi.org/10.2478/s11532-012-0090-6.

[7] A. S. Verma, "Study of electrical properties of ytterbium", The African Physical Review, 3, 11 (2009).

[8] C. M. Varma, “Mixed-valence compounds”, Reviews of Modern Physics, 48, 219 (1976). https://doi.org/10.1103/RevModPhys.48.219.
[9] S. Soni, M. Azad, K. K. Choudhary and N. Kaurav, “Structural phase transition and elastic behavior of WN”, AIP Conference Proceedings, 2100, 020085 (2019). https://doi.org/10.1063/1.5098639.
[10] D. Varseny, R. Kinge, P. Sharma, N. Karurav and R. K. Singh, “High pressure phase transformation and elastic behaviour of ZnX semiconducting compound”, Indian Journal of Pure & Applied Physics 43, 939-951 (2005).