LATTICE DYNAMICAL STUDY OF THORIUM SULPHIDE

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ABSTRACT

Thorium sulfide (ThS) is a chemical compound composed of thorium and sulfur atoms, with the chemical formula ThS. It belongs to the class of sulfides. To understand the dimensional stability and thermal behaviour of thorium sulphide (ThS), a lattice dynamical research issued to investigate its vibrational characteristics. We study the density of states (DOS) and phonon dispersion in the 50–60 GHz frequency region using computational techniques. Important information about the stability of the ThS crystal structure are given by the phonon dispersion curves, namely the presence of imaginary phonon frequencies that point to dynamical stability. We identify the major modes of vibration and their contributions to the thermodynamic properties of ThS through studying the phonon density of states.Van der Waals' three-body force shell model is used in this study to theoretically investigate the lattice dynamical behaviour of (ThS...). Elastic constants, pressure derivatives, dispersion relation curve, combined density of states, equation of state, and specific ultrasonic properties of the ThS are among the parameters for which calculated values are gave.The stability of the structure and vibrational properties of thorium sulphide are now better known by lattice dynamical study, which provides the way to its effective application in a range of technological uses, from nuclear reactors to the production of creative materials.

Keywords: lattice, dynamics, thermal, vibrational

INTRODUCTION

Thorium sulphide (ThS) lattice dynamical study examines atomic-level vibrational properties and structural stability of this molecule. A crystalline material known as thorium sulphide is made up of atoms of thorium and sulphur structured in a particular crystal lattice form. Because various scientific and technological applications, from nuclear energy to materials science, a knowledge of its lattice dynamics is important.

Lattice dynamical study related to the vibrational properties in a crystal lattice. These vibrational properties also knows as phonons which play a important role in describing the mechanical, thermal and electronic properties. With studying of vibrational properties like density of states, phonon dispersion and other vibrational properties researchers may learn knowledge about the thermal conductivity, specific heat capacity and stability of materials such as thorium sulphide.

Theory of lattice dynamics

- Lattice Dynamics: Lattice dynamics is the study of the collective motions of atoms within a crystal lattice. The periodic arrangement of atoms or ions in a solid material is called a crystal lattice.

- Harmonic Approximation: In lattice dynamics, atoms within a crystal lattice are commonly thought of as point masses connected by springs. Since the interatomic forces are assumed to be harmonic, a quadratic function can be used to approximate the potential energy in this approximation.

- The interatomic forces in the crystal lattice are represented by a matrix in the dynamical matrix. It links all of the atoms' lattice displacements to the forces acting on them individually. It is possible to calculate the frequencies and modes of lattice vibrations, or phonons, by diagonalizing the dynamics

Crystal geometry of Thorium sulphide:
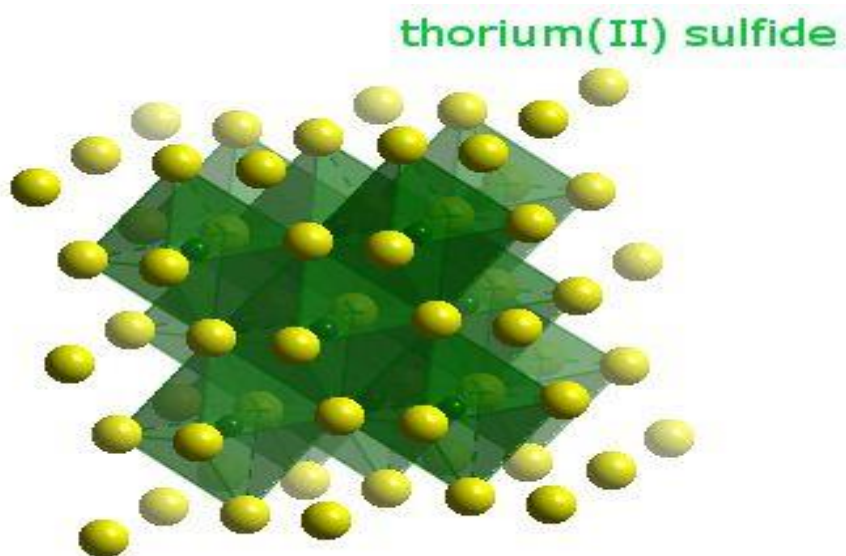
The face-centered cubic (FCC) structure, which is expressed by the space group "Fm3m" in the cubic crystal system in which ThS crystal locates. According to this space group, ThS has a cubic unit cell, with atoms arranged in the centre of each cube's face as well as its corners.

The length of the cube's edges, or a, is the only lattice specific that can properly define the unit cell parameters of ThS. Six sulphur atoms surround each thorium atom in the unit cell, forming an octahedral structure due to the location of atoms inside the cell. Six thorium atoms are connected with each sulphur atom in the same way. This arrangement provides a very symmetrical, highly packed structure.

ThS's octahedral coordinate geometry, cubic unit cell, and crystallographic symmetry contribute to the material's strength and stability. Understanding these structural properties is important for understanding the properties and behaviours of ThS in various applications such as temperature, pressure, and radiation.

Space group   Fm3m

Coordination geometry   Octahedral

Density function theory(DFT):

A computer quantum mechanical method called density functional theory (DFT) is used to study the electronic structure of atoms, molecules, and solids. a study of the electron density distribution, it provides a correct and effective method for calculating a number of characteristics, such as total energy, electronic density, and chemical reactivity. DFT is widely used in materials science and other fields
because it gives a useful method for studying difficult structures.

Van der Waals Potentials:

Van der waals potential , is also known as van der waals interaction potential is a model shows how the distance between two neutral atoms or molecules impacts the interaction energy between them. This attraction has a different nature, and it comes from the relationship of electron velocity between different atoms. If other atoms are present, each atom's electrons move close to the nucleus, forcing the atom to become an electric dipole. The van der Waals interaction potential is the sudden dipole moment of a closed shell atom that generated dipole moment on a comparable atom and interaction energy this arising. Van der waals interaction (VWI) potential is denoted by $\Phi^{v}(r)$.

Many- Body Potential:

It is well-known that the ions undergo some overlap during lattice vibrations, leading to bending of their electron shells. Charge moves between the overlapping nearby ions as an effect of this action. The long range many body interaction (MBI), of which the three body interaction (TBI) is the most important
component, occurs when these transferred charges interact with all other charges of the lattice with the related coulomb field.
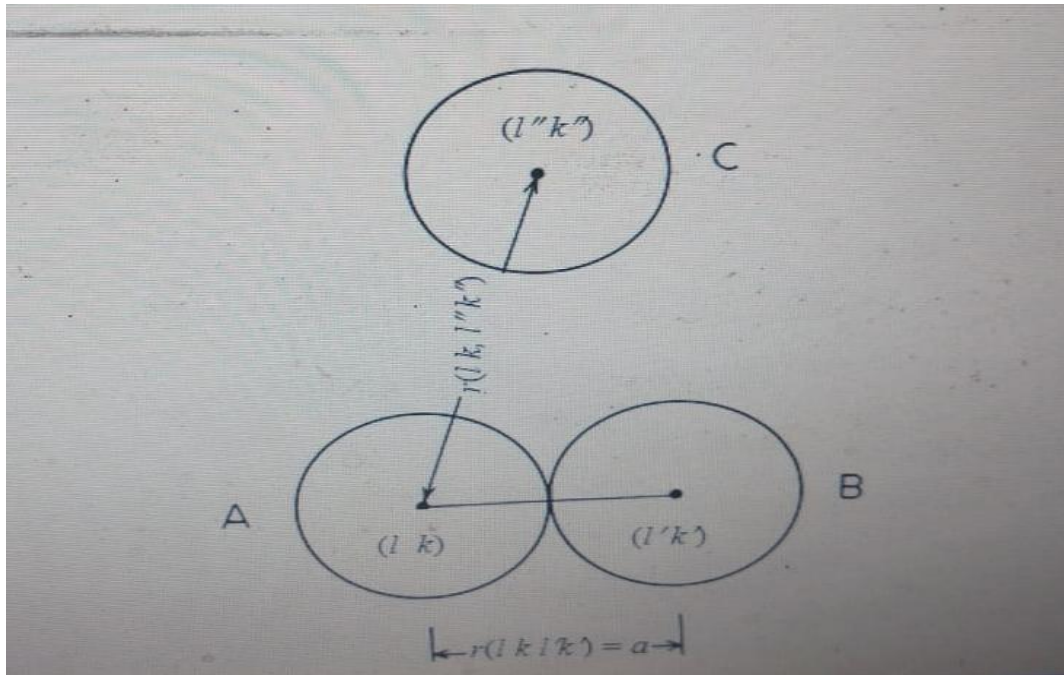
THREE- BODY INTERACTION

FIG- The electron charge clouds of the two nearby ions, A and B, interact as the two get closer to one another, changing their own net charges. Similarly, the third distant ion C affects A and B's ionic charges and produces a three-body force on them.

Equation for crystal potential per unit cell expressed as:

$$\Phi = \Phi^C + \Phi^R + \Phi^{TBI} + \Phi^{VWI}$$

Equation for vibrational properties:

$$(\mu\omega_L^2)_{q=0} = R_0' + \frac{(z'e)^2}{Vf_L}\frac{8\pi}{3}\left(1 + 12Z_m^{-2}Z_{r0}f_0'\right)$$

$$(\mu\omega_T^2)_{q=0} = R_0' - \frac{(z'e)^2}{Vf_T}\frac{4\pi}{3}$$

Rigid Shell Model (RSM)

Since Thorium sulphide (ThS) has potential uses in a number of areas, such as solid-state physics, materials research, and nuclear technology, it is a compound that is of great importance. Clarifying ThS's thermal, mechanical, and electrical properties requires an understanding of its lattice dynamics. The rigid shell model is one of the most simple but useful theoretical models for studying lattice dynamics. In the present paper, we study the lattice dynamics of thorium sulphide using the rigid shell model.

Theoretical Basis of the Rigid Shell Model:

The display of atoms within the crystal lattice is made simpler by the rigid shell model. It ignores the complex electronic structure and interatomic bonding interactions, treating each atom as a point mass in its equilibrium location. Atomic interactions are usually represented as harmonic oscillators, with quadratic terms surrounding the equilibrium locations describing the system's potential energy. The phonon frequencies can be computed using this harmonic approximation, which is essential for understanding the crystal lattice's vibrational behaviour.

Application of the Rigid Shell Model in Thorium Sulphide:

The rigid shell model provides important light on the lattice dynamics of ThS. Using the harmonic approximation, researchers can calculate the density of states, phonon dispersion relations, and other vibrational features by taking advantage of the interactions between thorium and sulphur atoms inside the crystal lattice. These computations help in the prediction of ThS's mechanical stability, specific heat capacity, and thermal conductivity at various pressure and temperature levels.

Rigid Ion Model (RIM):

Because thorium sulphide (ThS) has potential uses in a number of fields, including materials science and nuclear technology, there is a lot to examine in study it. Having an understanding of ThS's structural and dynamical features is important. A useful theoretical tool for understanding the behaviour of the crystal lattice of ThS is the rigid ion model. We cover basic concepts, uses, and results of the rigid ion model in ThS .

Theoretical Foundation of the Rigid Ion Model:

According to the rigid ion model, the negatively charged (anions) and positively charged (cations) in a crystal lattice are stable and show rigid behaviour. This model treats the ions as stable and concentrates only on their interactions, which simplifies the study of crystal formations. ThS is a compound in which sulphur atoms (S) function as (anions) and thorium atoms (Th) as (cations). The general stability and structural characteristics of ThS are explained by the rigid ion model, which takes into the Coulombic interactions between these ions and the surrounding electron cloud.

Structural Properties of ThS Under the Rigid Ion Model:

Th and S ion interaction and ordering inside the crystal lattice can be used to look at the structural properties of ThS under the rigid ion model. The rigidity and stability of the crystal structure of ThS are largely dependent on the pairing number, bond lengths, and angles of the Th and S ions. The equilibrium areas and geometric properties of ThS are very correctly predicted by the rigid ion model, which takes into the electrostatic interactions between the ions and the lattice energy related to their structure.

Vibrational Behavior and Phonon Modes:

While the rigid ion model considers ions as fixed groups, it can be extended for studying the ThS crystal lattice's vibrational motion. The model allows the calculation of phonon modes and related frequencies by adjusting for tiny displacements of ions from their equilibrium positions. These phonon modes provide insight on the mechanical and thermal characteristics of ThS by representing the collective vibrational movements of the ions inside the lattice. Also, the rigid ion model makes it easier to understand experimental methods that study the vibrational modes of ThS, like infrared and Raman spectroscopy.

Three-Body Force Shell Model (TSM):

Studying how atoms interact with one another inside a crystal lattice is important for studying materials at the atomic level. There are different force model are used to study the interaction between the pair of atoms. But in material where three or more atoms may interact with one another at the same time, these models fall short of representing the atomic interaction in materials. The three-body force shell model (TFSM), an idea for researching atomic interactions outside coupled forces, was developed in order to get overcome this drawback. In this article, we study the concepts, procedures, and applications of the TFSM in physics and materials science.

Introduction to the Three-Body Force Shell Model:

A theoretical structure called the TFSM is used to explain how atoms interact in a crystal lattice while including the combined effect of three or more atoms. Higher-order interactions are taken advantage of by the TFSM in opposed to paired force models, which only take into account interactions between pairs of atoms. This lets for a more thorough understanding of atomic behaviour in materials. The electron charge clouds of the two nearby ions, A and B interact as the two get closer to one another, changing their own net charges. Similarly the third distant ion C affects A and B's ionic charges and produces a three- body force on them.

Principles of the TFSM:

Three-body potentials, which describe the energy related to the arrangement of three atoms inside a crystal lattice, are the basic components of the TFSM. Generally generated by direct observation or quantum mechanical

computations, these potentials describe the interactions between all possible combinations of three atoms. Three-body interactions are included into the TFSM to give a more realistic picture of atomic behaviour in materials.

Methodological Approaches:

Many computational methods are used to execute the TFSM, depending on the specific application and system scale being studied. The electronic structure and atomic energies are frequently obtained by density functional theory (DFT) calculations, which later serve as input to build the three-body potentials. The movements of the atoms inside the crystal lattice may then be examined using molecular dynamics (MD) experiments, which enables physicists to look into how three-body interactions affect the characteristics of materials.

Ultrasonic properties

The term "ultrasonic properties" describes a wide range of features and events related to ultrasonic waves, which are sound waves with frequencies greater than the maximum limit of human hearing, typically above 20 kHz. The behaviors and effects that ultrasonic waves display as they move through various materials and interact with their surroundings are covered by these characteristics, which are very different. Understanding these features is necessary for maximizing the potential of ultrasonic technology in various fields like engineering, materials science, and medicine.

Several important ultrasonic properties are:

Propagation: Materials' density, elasticity, and other physical characteristics effect how ultrasonic waves flow through them. These factors affect the ultrasonic wave's propagation speed, symmetry, and dispersion. Important elements of propagation qualities involve processes like attenuation, in which waves lose intensity as they pass through a medium as a result of absorption and scattering.

Reflection and Transmission: Ultrasonic waves can be absorbed, transmitted, or reflected when they get into interaction with irregularities within a medium or borders between various materials. For applications like non-destructive testing (NDT) and medical imaging, where reflection from internal structures provide important information about the material's quality or the internal structure of the body, an understanding of how ultrasonic waves behave at surfaces is important.

Absorption: Materials have the ability to absorb ultrasonic waves and change their energy from motion into other forms, like heat. The properties of the medium and the wave frequency have an effect on how it absorbs of ultrasonic energy. The ability of tissues to absorb ultrasonic waves can be used effectively in medical applications, such as focused heat of unwell tissues by ultrasound treatment.

Ultrasonic waves

Mechanical waves known as ultrasonic waves move through a material at frequencies that are higher than the upper limit of human hearing, usually more than 20 kHz. These waves have unique characteristics and are used in a wide range of industries, such as engineering, materials research, and medicine.

The high frequency of ultrasonic waves, that allows them to carry more energy and enter materials more effectively than audible sound waves, is one of their main characteristics. Due to this characteristic, ultrasonics are very helpful in applications like medical ultrasonography and non-destructive testing (NDT) in industrial settings requiring for correct imaging and sensing capabilities.

Sensors, which convert electrical energy into mechanical vibrations, are used to create ultrasonic waves. Usually made of piezoelectric materials, these sensors produce ultrasonic waves that travel through the surrounding medium when an applied voltage leads them to bend. The transducer's design defines the frequency of the waves it produces, which can be changed to fit a wide range of uses.

Ultrasound imaging in medical is one of the main uses for ultrasonic waves. Using this method, ultrasonic vibrations enter the body and reflect against interior organs and tissues. The internal structures of the body can be observed from deep through studying the length of time it takes for the waves to return and the magnitude of the reflected signals. Ultrasound imaging is a common diagnostic tool for many health conditions, such as monitoring heart function, finding cancer, and monitoring pregnancy.

Types of ultrasonic waves

Different types of ultrasonic waves can be classified by their frequency range, application, and method of transmission. Some common forms of ultrasonic waves are as follows:

Longitudinal Waves: The movement of the particles in these ultrasonic waves is opposite to the direction of wave propagation, making them the most common form. Particles oscillate back and forth along the same axis as the wave moves along in longitudinal waves. These waves are frequently used in industrial testing, material analysis, and medical imaging.

Transverse Waves: Particle movement in transverse waves occurs perpendicular to the wave's propagation direction. Compared to longitudinal waves, these waves are less common in ultrasonics, but they can still occur in certain situations. Usually, transverse waves are used in specific applications like surface wave monitoring methods.

Surface Waves: Surface waves travel across the boundary, state, between a solid and a liquid or gas, between two distinct materials. Instead of hitting the mass of the substance, these waves move over its surface. In non-destructive

testing (NDT) applications, surface waves can be used, particularly for surface examination and defect or gap detection.

Ultrasonic analysis of different parameters:

An important variable in the development of materials is ultrasonic velocity. Anisotropic solids impact how ultrasonic waves propagate because of strains in the <100>, <110>, and <111> directions. There are three types of propagation for ultrasonic waves' velocity when they pass through a medium: longitudinal acoustical (V_L) and shear acoustical (V_{S1}, V_{S2}).The expression for VL, Vs1 and Vs2 are given:

Along the <100> crystallographic direction:

$$V_L = \sqrt{C_{11}/d}$$

$$V_{s1} = V_{s2} = \sqrt{C_{44}/d}$$

Along the <110> crystallographic direction:

$$V_L = \sqrt{(C_{11} + C_{12} + C_{44})/2d}$$

$$V_{s1} = \sqrt{C_{44}/d}$$

$$V_{s2} = \sqrt{(C_{11} - C_{12})/d}$$

Along the <111> crystallographic direction:

$$V_L = \sqrt{(C_{11} + 2C_{12} + 4C_{44})/3d}$$

$$V_{S1} = V_{S2} = \sqrt{(C_{11} - C_{12} + C_{44})/3d}$$

Table.1-Input data and model parameters for ThS C_{ij} (in 10^{12} dyne cm2),v (in THz), r_0 (in 10^{-8} cm),α_i (in 10^{-24} cm)

C_{11}	C_{12}	C_{44}	R0	A_{12}	B_{12}	d_1	d_2
3.0766	0.5015	0.2761	2.8425	3.0766	0.5015	0.2761	2.8425

This are the input data and model parameters for ThS. Now using these input data we calculated the ultrasonic velocities of V_L, V_{S1}, V_{S2} and V_D

Table-2 Calculated Orientation dependent ultrasonic velocities V_L, V_{S1}, V_{S2} and V_D (in $10^3 ms^{-1}$) of ThS at room temperature

Material Orientation	V_L (Longitudinal Acoustical)	V_{S1} (Ist Shear acoustic	V_{S2} (2nd Shear acoustic)	V_D (Debye Temperature)
<100>	0.2402	0.0719	0.0719	0.0819
<110>	0.1735	0.0719	0.2198	0.1002
<111>	0.1039	0.0771	0.0771	0.0829

Longitudinal Acoustical (V_L):

The field of acoustics referred to as longitudinal acoustics focuses on the study of longitudinal waves in materials, especially in solids, liquids, and gases. Particle movement in these waves occurs parallel to the direction of wave propagation, i.e., the particles oscillate along the same axis as the wave moves. Many fields, including physics, engineering, materials science, and medicine, depend on an understanding of longitudinal acoustics.

The nature of longitudinal waves itself is one of the basic ideas in longitudinal acoustics. The alternating regions of compression and rarefaction within the medium that longitudinal waves move through define their features. Particles oscillate parallel to the direction of wave propagation in a longitudinal wave, moving apart in rarefaction zones and closer together in compressing regions. The wave can propagate because of the energy transferred through the medium by this steady motion.

A medium's longitudinal wave speed is defined by the density, elasticity, and elasticity of the material. Longitudinal waves normally proceed more quickly in solids than through liquids and even quicker through gasses. Variations in temperature, pressure, and the number of impurities or problems in the material can all affect this speed.Longitudinal waves are important for many practical uses. For example, longitudinal waves are frequently used in non-destructive testing (NDT) to check the interior structure of materials for defects or errors without causing damage. Defects like as cracks, voids, and inclusions can be detected, diagnosed, and characterised by producing and detecting longitudinal waves with the use of specialized tools such ultrasonic instruments.

The use of longitudinal waves in medical ultrasound imaging is another important application. High-frequency longitudinal waves are injected into the body during ultrasound imaging, where they are reflected off interior organs and tissues. Through the analysis of the echoes generated by these waves, accurate pictures of the interior of the body may be obtained. This allows doctors to track growth during pregnancy, diagnose a variety of medical disorders, and guide other surgeries.

Shear acoustic (V_S):

Particle motion perpendicular to the direction of wave propagation describes shear acoustic waves, commonly referred to as transverse waves or shear waves. Shear waves cause motion perpendicular to the direction of propagation, resulting in side-to-side or up-and-down particle oscillation, in contrast to longitudinal waves, which show particle displacement parallel to the direction of propagation.Shear waves can travel through gases, liquids, and solid objects, but their properties and behaviour change according to the medium. Shear waves propagate more slowly in solids than longitudinal waves, and they are affected by the density, Poisson's ratio, and shear modulus of the material. Shear waves can be generated and modified for a wide range of applications, including non-destructive testing (NDT),

Characteristics of Shear Waves:

Particle Motion: In shear waves, the direction of wave propagation is perpendicular to the motion of the particles within the medium. The term "shear waves" refers to the shearing or sliding of material layers in relation to one another in this action.Propagation Velocity: Shear wave velocity is dependent upon the mechanical properties of the medium, including density and shear modulus. Shear waves normally propagate more slowly in solid materials than longitudinal waves.Wave Polarization: Particle motion in shear waves is perpendicular to the direction of wave propagation, an effect known as polarization. Shear waves interact with materials differently than longitudinal waves because of this polarization.

The lattice dynamical study of thorium sulphide provides significant updates of its thermal, phonon dispersion, and strength. Phonon studies offer an in-depth knowledge of its vibrational behavior and thermal conductivity through computational methods In this by use of theatrical model van der Waals three body force shell model, that will be used for calculation of different parameters. Kknowledge of the different characteristics of thorium sulphide, provide important information about its uses in materials research and nuclear technology. Additional theoretical developments and experimental findings are necessary for reaching its potential and overcome difficulties in practical use. The following parameters are calculated by help different theoretical model like-Elastic constant, Combined density of states, Debye temperature, Ultrasonic properties of the material, Pressure derivatives.

Phonon dispersion:

The concept of phonon dispersion comes from solid-state physics and describes how lattice vibrations behave in a crystalline material. Understanding the different mechanical, electrical, and thermal properties of materials is important. Like photons, which describe quantized light energy, phonons basically represent quantized lattice vibrations. The energy and momentum of a phonon define its features within the crystal lattice, just as the energy and momentum of a photon affect its behaviour.

A complete analysis of the phonon energy variation with momentum over the Brillouin zone, the fundamental unit of the inverse lattice of the crystal, may be found in phonon dispersion relations. Scientists can learn more about thermal conductivity, thermal expansion, and other important material qualities by studying these connections.The regularity of the crystal lattice is critical to phonon dispersion. A simple representation of the lattice consists of a collection of atoms connected by originates where each atom would represent a minimum of potential energy. These atoms change about their equilibrium locations in response to perturbations, such as thermal energy, producing waves of energy called phonons.

For simplicity, let's examine at a one-dimensional lattice to understand phonon dispersion. The dispersion relation explains the relationship between the wavevector (momentum) and the frequency (energy) of phonons. Every atom in a basic monoatomic 1D lattice is the same, and there is only one form of phonon. In this case, the dispersion relation is linear, and its slope is equal to the force constant divided by the atomic mass square.

Brillouin Zone:

Understanding the electrical and vibrational characteristics of crystalline materials required an understanding of the Brillouin zone, an important concept in solid-state physics and crystallography. It is a special geometric design in open space that represents the periodicity of the crystal lattice and is named after the French physicist Leon Brillouin.The atoms are arranged in a crystalline solid in a continuing, three-dimensional pattern called a lattice. The unit cell of the inverse lattice, which is the real-space lattice's Fourier transform, is known as the Brillouin zone. The set of all wavevectors that can be added to a reciprocal lattice vector without leading the lattice to break describes it.

Elastic constant:

The mechanical behaviour of materials under the action of external forces or movement is described by features called elastic constants. These constants offer important information on the material's stiffness, elasticity, and capacity of supporting stress without completely deformed. For structural analysis, material selection, and engineering design in a variety of industries, an understanding of elastic constants is important.

Young's modulus, additionally referred to as the tensile modulus or the modulus of elasticity, is one of the most frequently discussed elastic constants. The ratio of stress to strain in a material under compressed or tensile loading can be measured by the Young's modulus. It shows how resistant a material is to deformation along its length when subjected to axial stresses. The ratio of axial stress (force per unit area) to axial strain (change in length per unit length) within the region of elastic deformation is known as Young's modulus.

In addition, a basic elastic constant called the bulk modulus explains the way a material reacts to hydrostatic compression or expansion. The resistance of a substance to volume changes under uniform pressure is measured by the bulk modulus. Within the range of elastic deformation, it is the ratio of the hydrostatic stress (pressure) to the

volumetric strain (change in volume per unit volume). For materials like liquids, gases, and porous solids that are exposed to fluid pressure, the bulk modulus is very important.

$$C_{11} = \frac{e^2}{4r_0^4}\left[0.7010Z_m{}^2 + A_{12}/6 + B_{12}/3 + 5.4283\,\xi'^2\right]$$

$$C_{12} = \frac{e^2}{4r_0^4}\left[-0.6898Z_m{}^2 + A_{12}/6 - 2B_{12}/3 + 5.4283\,\xi'^2\right]$$

$$C_{44} = \frac{e^2}{4r_0^4}\left[-0.3505Z_m{}^2 + A_{12}/6 + B_{12}/3\right]$$

Equation for the elastic constant.

C_{11}, C_{12} and C_{44} are components of the elastic rigidity tensor, which is a crucial parameter in explaining the mechanical behaviour of crystalline materials, particularly in the context of isotropic elasticity, in solid-state physics and materials science. The research study conducted by notes, which makes the formulation of the elastic stiffness tensor simpler, frequently makes use of these values.
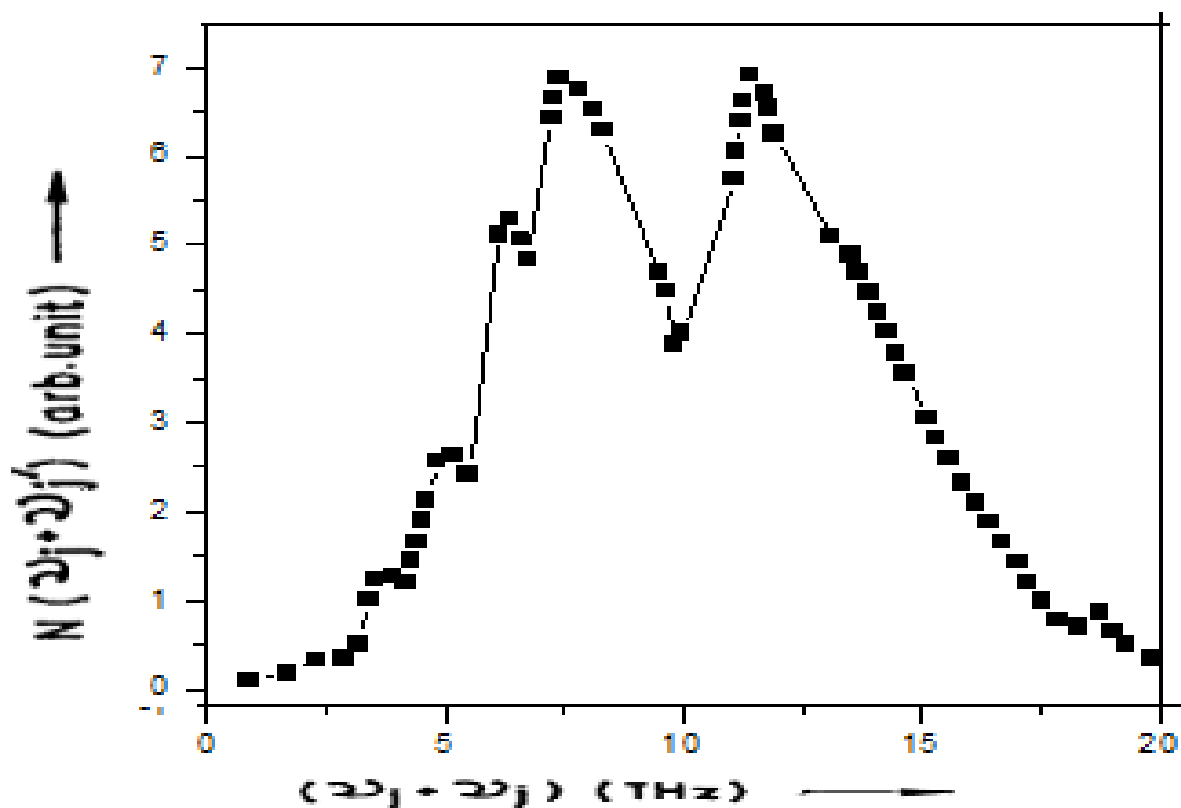
Combined density of states:

In the fields of condensed matter physics and materials science, the combined density of states (or CDOS) is a basic idea that offers important insights into the electrical structure and characteristics of materials. Considering both the electronic states connected with the valence band (occupied states) and the conduction band (unoccupied states), it represents the density of possible electronic states per unit energy range. Understanding CDOS is crucial for planning and analysing different optical and electrical properties of substances.

An energy range known as the bandgap, which shows the absence of occupied electronic states, characterizes the electronic structure of many materials, including semiconductors and insulators. The conduction band, which has free states that energetic electrons can occupy, is located above this bandgap. The valence band, which is electron-rich, is located below the bandgap. The CDOS gives a complete picture of the electronic states that are possible in the material by considering note of both the valence and conduction bands.In mathematical terms, the CDOS can be defined as the total of the valence band's density of states (DOS) and the conduction band's DOS. Within each band, the arrangement of electronic states as a function of momentum and energy is described by the DOS. As an example, the DOS is constant within each band in a basic model like the free electron gas model. However, because of things like band curvature, band mixing, and electron-electron interactions, the DOS can behave deeply in real materials.

Computation:

Combined Density of States (CDOS) curve provides information about the density of electronic states in a material as a function of energy. The experimental results for Θ_D were obtained on basis of C_P measurements. The analysis for knowing occupied states or occupation of electron, the combined density of states CDOS measurement done. The CDOS is plotted in Figure 1. It provides valuable information about distribution of energy states and the availability of electronic states of different energy levels.

The density of states of a system indicates the number of modes per unit frequency range in dense matter and solid-state physics. Peaks on the combined density of states (CDOS) graph indicate particular electronic transitions or material energy levels. These transitions are caused by photons, electrons, or other excited states that the material's electrons absorb or emit. Peaks in the CDOS spectrum indicate the presence of electronic states at specific energy levels, which are connected to a range of physical processes.

Low peaks in a combined density of states graph usually indicate electronic transitions or energy levels with lower densities of states or lower probability of existence. These transitions relate to processes that are less positively charged or to electronic states that are less populated in the material.
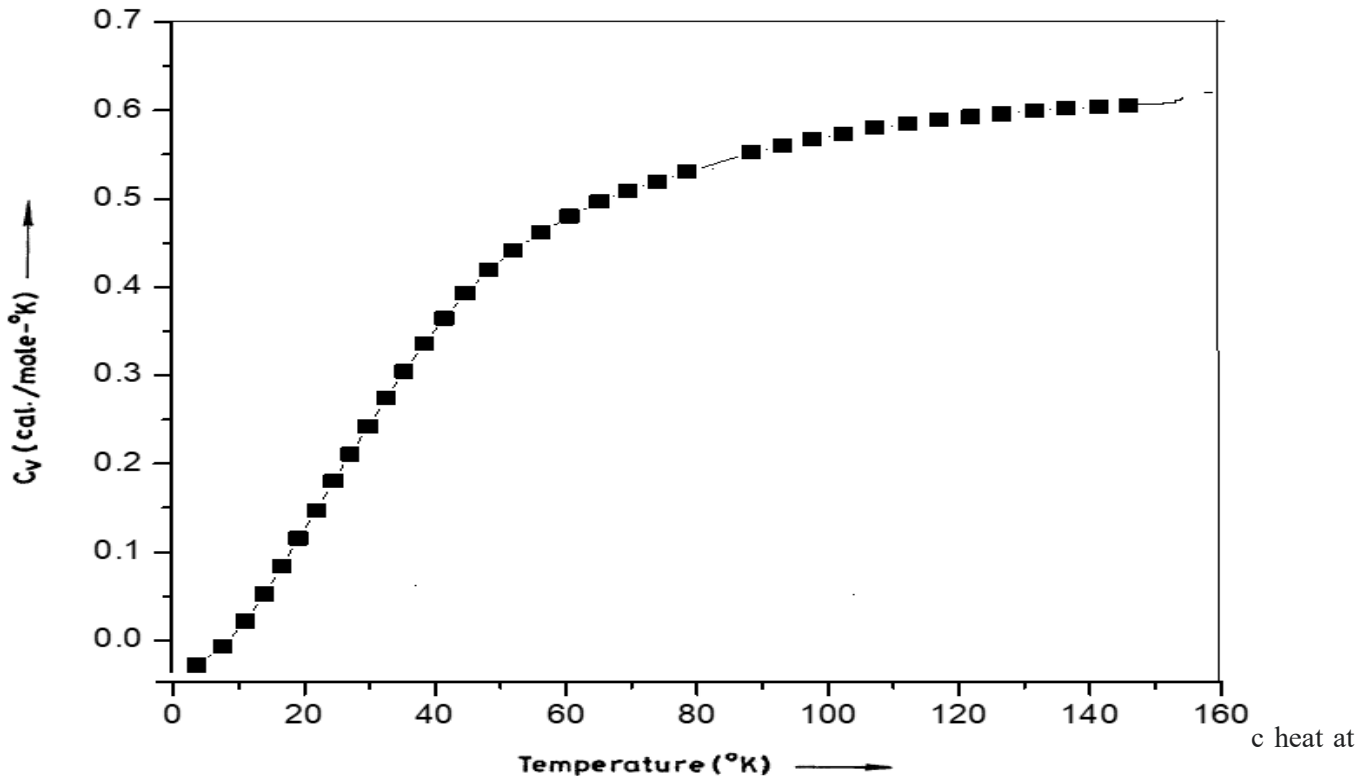
c heat at constant volume) versus temperature graph. The amount of heat needed to raise a unit mass of a substance's temperature by one degree Celsius (or Kelvin) at constant volume is known as the specific heat capacity, or Cv. At low temperatures, contributions from lattice vibrations, or phonons, generally lead the specific heat capacity. Because of the increased thermal energy and vibrational motion of the atoms in the lattice, the specific heat capacity usually displays a Debye-like behaviour as temperature rises.

The specific heat capacity may contain electronic contributions in addition to lattice contributions, particularly at higher temperatures where electronic excited states become important. These electronic contributions may result from other electronic transitions occurring within the material or from thermal excited states of electrons across the bandgap.Phase transitions in the material may be indicated by variations in the graph's slope or discontinuities (Cv versus temperature). A phase transition, such as a structural, magnetic, or superconducting phase transition, may be represented as a peak, shoulder, or gap in the specific heat curve.

Debye temperature:

An important quantity in solid-state physics, the Debye temperature is named for the physicist Peter Debye and describes the average vibrational energy of atoms or molecules in a crystalline substance. It is important for understanding the different mechanical, electrical, and thermal properties of solids. When studying lattice vibrations and the behaviour of phonons—quantized vibrational modes in the crystal lattice—the concept of Debye temperature

is particularly important.Debye temperature, in its most basic form, is the temperature scale at which the solid's phonon density of states is completely full. Stated differently, it designates the temperature below which all phonons, or vibrational modes, contribute to the material's thermal characteristics. Higher energy phonon modes start to fill up above extra thermal energy, which changes the behaviour of the material.

The Debye model of lattice vibrations, which is based on the mathematical concept that the solid behaves as a continuous elastic media, is frequently used to define the Debye temperature. The average vibrational energy of the phonons within the crystal lattice is related to the Debye temperature in this model, and the phonon density of states can be approximated by a characteristic Debye function.

For a given material, the Debye temperature can be determined or predicted using a variety of theoretical models and experimental methods. In certain cases, tests like neutron scattering, infrared spectroscopy, or specific heat measurements allow for direct measurement. In addition, the elastic constants, lattice parameters, and other physical characteristics of the material can be used to calculate the Debye temperature.

Result:

In this manuscript the input data and other calculated parameters are reported for (ThS) in the Table-1, Calculated Orientation dependent ultrasonic velocities in Table-2 using the values of input constants & parameters . The CDS analysis is helping to understand the sensitivity up to the atomic-level stresses and microstructure. By use of CDS curve electrical conductivity with their related effects can be study, curve is shown in Figure-1. It is observed that at higher temperature's convergence of C_V to the Dulong–Petit's limit. Overall, the molar heat capacity graph provides valuable insights into the thermal behaviour of substance and its ability to store and transfer of heat energy at different temperatures shown in Figure-2.Vital role of ultrasonic velocity in the characterization of (ThS) can be observed. The propagation of ultrasonic waves depends on the strains along the <100>, <110>, <111> directions are calculated.

Conclusion:

The thermophysical and ultrasonic properties with lattice dynamical calculations of ThS which based on different available parameters is successfully reported. By the use of experimentally reported value of the input data table-1 and the Orientation dependent ultrasonic velocities reported theoretically in table-2. In the present study in lower symmetry. ThS shows uncertainty as well as distortion structure that showed good agreement, while at higher temperature. slight disagreement occurred. which deduced that the incorporation of van der Waals interactions are essential and important. The Complete thermophysical property of ThS are theoretically reported, which have agreed with expt. reported data. . The present model has successfully used with various researchers and reported. lattice dynamical properties of different halides & semiconductor materials. So, in complete lattice dynamical study of (ThS) compound the inclusion of VWI are very essential.

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