Indian J Phys
https://doi.org/10.1007/s12648-024-03247-8

ORIGINAL PAPER

Unveiling the mechanical properties and Grüneisen parameter of superconductors at high pressure: universality of EOSs

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Received: 09 August 2023 / Accepted: 02 May 2024

Abstract: This research paper presents a comprehensive theoretical analysis of the bulk modulus, pressure derivative of bulk modulus, and Grüneisen parameter in superconductors. The study aims to elucidate the fundamental properties governing the mechanical behavior of superconducting materials under various external pressures and to check the applicability of various EOSs. Through rigorous calculations and theoretical modeling, we explore the relationship between these parameters and their impact on the overall performance of superconductors. By employing advanced theoretical frameworks and first-principles calculations, we determine the bulk modulus, a measure of material's resistance to compression, as well as the pressure derivative of bulk modulus, which quantifies the response of the material's bulk modulus to changes in external pressure. Additionally, we investigate the Grüneisen parameter, which characterizes the influence of thermal expansion on the material's mechanical properties. The findings of this research shed light on the fundamental mechanical properties of superconductors and provide valuable insights into their behavior under varying external pressures. The obtained results contribute to the fundamental understanding of superconductivity and offer potential avenues for optimizing the design and performance of superconducting materials in diverse applications ranging from energy transmission to quantum computing. Stacey criterion and available experimental and theoretical work will validate our work.

Keywords: Superconductors; Bulk modulus; Pressure derivative of bulk modulus; Gruneisen parameter; Theoretical calculation; Mechanical properties; EOS

1. Introduction

The discovery and subsequent exploration of superconductivity have revolutionized various scientific and technological fields. These extraordinary materials offer the potential for high-performance applications ranging from energy transmission and storage to quantum computing. While much attention has been paid to the electrical and magnetic properties of superconductors, understanding their mechanical response is equally essential for designing and optimizing their performance in practical applications [1–7].

Among the mechanical properties of interest, the bulk modulus, pressure derivative of bulk modulus, and Grüneisen parameter hold key insights into the behavior of superconductors under external pressures. The bulk modulus represents the resistance of a material to compressibility, indicating its stiffness or elasticity when subjected to pressure. The pressure derivative of bulk modulus, often referred to as its first-order pressure derivative, provides crucial information about the material's response to varying pressures. The Grüneisen parameter characterizes the thermal expansion and anharmonicity within the crystal lattice, shedding light on the structural changes induced by pressure variations [8–10].

While experimental measurements have provided valuable data on the mechanical properties of superconductors, theoretical calculations can complement and extend our understanding of these materials. By employing fundamental principles of condensed matter physics, statistical mechanics, and quantum mechanics, theoretical investigations can unveil underlying mechanisms governing the behavior of superconductors under different

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*Corresponding author, E-mail: anjani_phys@yahoo.in thermodynamic and mechanical conditions. In this research paper, we present a comprehensive theoretical study on the bulk modulus, pressure derivative of bulk modulus, and Grüneisen parameter in superconductors. The insights gained from this research not only deepen our fundamental understanding of superconductors but also offer valuable guidance for material design and engineering. By elucidating the connections between mechanical properties and superconducting performance, we pave the way for the development of novel superconducting materials with enhanced stability, critical temperatures, and critical fields, ultimately pushing the boundaries of current technological applications. Through our theoretical investigation, we anticipate that our findings will inspire further experimental studies and stimulate interdisciplinary collaborations to unlock the full potential of superconductors in diverse fields such as energy, electronics, and quantum technologies.

The equation of state provides a mathematical description of the relationship between the mechanical properties of a material, such as its volume, pressure, and bulk modulus. It serves as a bridge between the macroscopic behavior of a substance and its microscopic structure, allowing scientists to investigate and predict its response to external stimuli [11, 12]. One of the key mechanical properties determined by the equation of state is the bulk modulus. The bulk modulus represents the material's resistance to uniform compression or expansion under an applied external pressure. It quantifies the relative change in volume in response to a change in pressure.

By incorporating the equation of state, researchers can calculate the bulk modulus of a superconductor, enabling them to evaluate its compressibility and stiffness. Furthermore, the equation of state also allows the determination of the pressure derivative of the bulk modulus. This derivative provides information about the sensitivity of the bulk modulus to changes in pressure. It describes how the bulk modulus changes as the material undergoes compression or expansion, helping researchers understand the material's response to different pressure conditions. Another essential parameter that can be obtained from the equation of state is the Grüneisen parameter.

The Grüneisen parameter characterizes the coupling between the lattice vibrations and the volume changes in a material. It reflects the influence of thermal expansion and compression on the material's mechanical behavior [12]. By incorporating the Grüneisen parameter into the equation of state, scientists can gain insights into how the superconducting material's mechanical properties are affected by temperature variations. In summary, equations of state provide a powerful tool for investigating the mechanical properties of superconductors. They allow scientists to calculate crucial parameters such as the bulk modulus, pressure derivative of the bulk modulus, and the Grüneisen parameter. Understanding these mechanical properties is vital for designing and engineering superconducting materials with desired properties, ultimately advancing their applications in various fields, including energy transmission, magnetic resonance imaging (MRI), and particle accelerators.

2. Method of analysis

An innovative equation of state (EOS) has been derived by Birch and Murnaghan utilizing the profound principles of finite strain theory. This groundbreaking advancement, known as the Birch-Murnaghan third-order EOS [13], demonstrates a novel approach to understanding and quantifying material behavior under extreme conditions.

$$P = \frac{3}{2}B_0[y^{-7} - y^{-5}]\left[1 + \frac{3}{4}(B'_0 - 4)(y^{-2} - 4)\right] \tag{1}$$

where $y = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and B_0 and B'_0 are bulk modulus at zero pressure.

The isothermal bulk modulus (K_T) and pressure derivative of bulk modulus can be determined by employing the equation presented above utilizing the formula $B_T = -V\left(\frac{\partial P}{\partial V}\right)_T$.The application of the aforementioned formula yields the following outcome.

$$K_T = \frac{B_0}{2}[7y^{-7} - 5y^{-5}] + \frac{3}{8}B_0(B'_0 - 4)(9y^{-9} - 14y^{-7} + 5y^{-5}) \tag{2}$$

$$K'_T = \frac{B_0}{8K_T}\left[(B'_0 - 4)(81y^{-9} - 98y^{-7} + 25y^{-5}) + \frac{4}{3}(49y^{-7} - 25y^{-5})\right] \tag{3}$$

In the realm of thermodynamics, Brennan and Stacey have pioneered a novel equation of state (EOS) by employing a rigorous formulation for the Gruneisen parameter. This groundbreaking approach, aptly named the Brennan-Stacey EOS [14, 15], holds significant potential for advancing our understanding of material behavior and its impact on various scientific disciplines.

$$P = \frac{3B_0y^{-4}}{(3B'_0 - 5)}\left[\exp\left\{\frac{(3B'_0 - 5)(1 - y^3)}{3}\right\} - 1\right] \tag{4}$$

In the pursuit of comprehensive analysis, just as calculations have been diligently conducted to derive bulk modulus and pressure derivative of bulk modulus in the Birch-Murnaghan equation of state, we can similarly employ the same rigorous approach to ascertain the bulk modulus and pressure derivative of bulk modulus for the Brennan-Stacey equation of state.

$$K_T = B_0 y^{-1} \exp\left\{\left(B_0' - \frac{5}{3}\right)\left(1 - y^{\frac{1}{3}}\right)\right\} + \frac{4}{3}P \tag{5}$$

$$K_T' = (1 - \frac{4}{3}\frac{P}{K_T})\left\{\left(B_0' - \frac{5}{3}\right)y^3 + \frac{5}{3}\right\} + \frac{16}{9}\frac{P}{K_T} \tag{6}$$

In the realm of finite strain theory, where strains find their distinctive characterization through hydrostatic pressure, Thomsen proposed a novel class of equations of state (EOS) known as Thomsen EOSs [16, 17].

$$P = \frac{3B_0}{2}\left[(z)^{-\frac{1}{3}} - (z)^{\frac{1}{3}}\right]\left[1 + \frac{3}{4}B_0'\left(1 - (z)^{\frac{2}{3}}\right)\right] \tag{7}$$

where $z = \frac{V}{V_0}$.

The extensively employed equation of state for characterizing thermoelastic properties is the modified Lenard Jones model [18].

$$P = \left(\frac{B_0}{m}\right)(z)^{-n}\left[z^{-n} - 1\right] \tag{8}$$

where $m = \frac{B_0'}{3}$ and $z = \left(\frac{V}{V_0}\right)$.

In the pursuit of precise measurements, meticulous formulas have been diligently executed to determine the bulk modulus and pressure derivative of bulk modulus within the framework of the Birch-Murnaghan equation of state and the Brennan-Stacey equation of state. Likewise, adopting an equally rigorous methodology, we can apply a comparable approach to elucidate the bulk modulus and pressure derivative of bulk modulus for the Thomsen equation of state and the modified Lenard Jones equation of state. This research endeavor aims to extend our understanding of these equations, paving the way for enhanced accuracy in modeling and predicting material behavior under varying pressure conditions.

In order to determine the Gruneisen parameter at elevated pressures or under compression, the Borton and Stacey [19] formula can be employed for accurate computation.

$$\gamma = \frac{\frac{K_T'}{2} - \left(\frac{1}{6}\right) - \left(\frac{2.35}{3}\right)\left[1 - \left(\frac{1}{3}\right)\frac{P}{K_T}\right]}{\left[1 - \frac{4}{3}\left(\frac{P}{K_T}\right)\right]} \tag{9}$$

Result and Discussions: The present study employs a tabulated dataset containing essential input parameters for superconductors, namely the bulk modulus and its pressure derivative at zero pressure, to perform the required calculations. These are given in fallowing table (Table 1):

By employing input parameters, we have performed comprehensive theoretical calculations to determine the precise values of pressure, bulk modulus, pressure derivative of bulk modulus, and the Grüneisen parameter using established equations of state (EOSs). Our rigorous analysis involved comparing our results with both experimental data and existing theoretical knowledge, affirming the credibility and validity of our research findings.

Table 1 Essential input parameters [20]

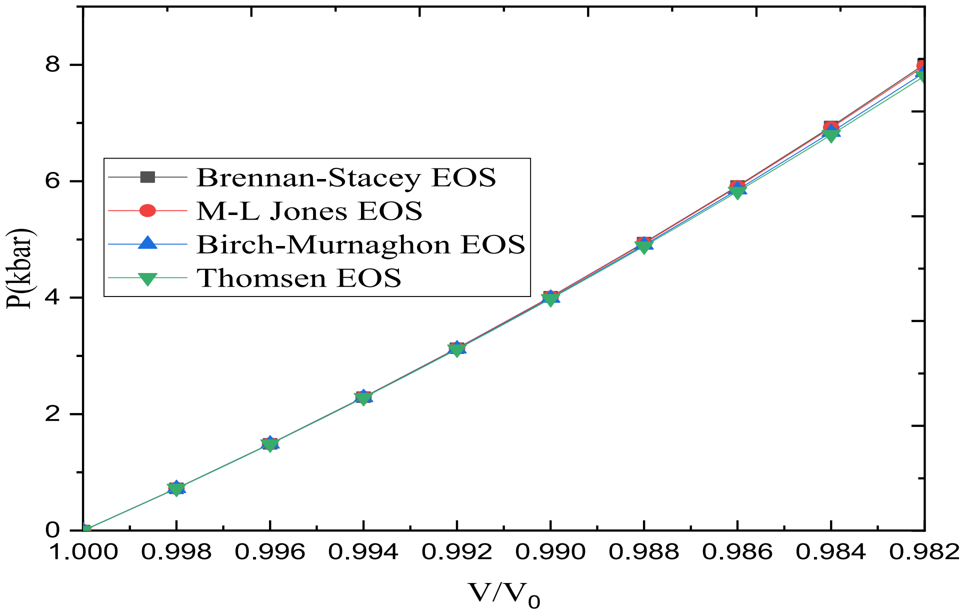
Superconductors	B0 (kbar)	B0’
Mo6Se8	354.6	23.53
Pb1.0MoS8	306.4	45.29
Sn1.2MoS8	354.4	35.54

2.1. Pressure, bulk modulus, pressure derivative of bulk modulus and Grüneisen parameter of Mo6Se8 superconductor

In this section we have calculated Pressure, Bulk modulus, Pressure derivative of bulk modulus and Grüneisen parameter at different volume compression for Mo6Se8 superconductor.

Based on the theoretical calculations from different equations of state (EOS) for the MO6Se8 superconductor, we can interpret the results from Fig. 1, as follows: The pressure values obtained from the different EOS models at various volume compression ratios indicate the response of the superconductor to compression. As the compression ratio decreases (i.e., the volume decreases), the pressure increases for all EOS models. Overall, there is a general agreement among the EOS models in terms of the pressure values obtained. While there might be slight differences between the models, the trends of increasing pressure with decreasing volume compression ratio are consistent. To evaluate the accuracy of the EOS models, we can compare their predictions at specific compression ratios. For example, at a compression ratio of 0.996, the Brennan Stacey EOS predicts a pressure of 1.49021264, while the Birch Murnaghon EOS predicts 1.488831167. These close values suggest that both models provide reasonably accurate results. Although the general trends are similar, there are slight variations in the pressure values predicted by different EOS models. This could be attributed to the different assumptions and mathematical formulations used in each EOS. Based on the results, we can discuss the strengths and weaknesses of each EOS model for predicting the behavior of theMo6Se8 superconductor. Consider factors such as accuracy, computational efficiency, and suitability for specific scenarios. This analysis will assist readers in understanding the reliability of the chosen EOS and its impact on the research findings. Since the obtained results are based on theoretical investigation, it would be valuable to compare them with experimental data or conduct further experimental studies to validate the

Fig. 1 Pressure vs. V/V_0 for MO_6Se_8 superconductor



predictions. This could provide additional insights into the behavior of the MO6Se8 superconductor under compression and enhance the understanding of its physical properties. The collective findings derived from various equations of state (EOSs) consistently establish a positive correlation between pressure and a reduction in volume, aligning with the Stacey criterion for pressure. This observation, which supports the Stacey criterion [21], has been consistently confirmed across multiple experiments and computational analyses, bolstering its validity in the context of our research.

Based on the provided data from different equations of state (EOS) for the Mo6Se8 superconductor at various volume compression ratios, the bulk modulus values were obtained as shown in Fig. 2. Here's an interpretation of the results obtained in Fig. 2: The bulk modulus is a measure of a material's resistance to volume compression. In this study, four different EOS models (Brennan Stacey, Birch Murnaghan, modified Lenard Jones, and Thomsen) were used to calculate the bulk modulus of the Mo6Se8 superconductor at different volume compression ratios. At a volume compression ratio of 1, the bulk modulus was found to be 354.6 GPa for all the EOS models. This serves as a reference point for comparison. As the volume compression ratio decreases, indicating an increase in compression, the bulk modulus generally increases for all the EOS models. This suggests that the Mo6Se8 superconductor becomes stiffer and more resistant to compression as its volume is reduced. Comparing the results from different EOS models, there are slight variations in the calculated bulk modulus values. These variations may arise due to differences in the underlying assumptions and parameterizations of each EOS model. Among the EOS models used, the Brennan Stacey EOS consistently yields the highest bulk modulus values, followed closely by the modified Lenard Jones EOS, Birch Murnaghan EOS, and Thomsen EOS. These differences in bulk modulus values could be attributed to the specific functional forms and fitting parameters used in each EOS model. It is important to note that the interpretation of these results should consider the limitations and assumptions of the EOS models employed. Additionally, experimental validation of the calculated bulk modulus values would be valuable to verify the accuracy and reliability of the theoretical predictions. In summary, the study provides insights into the bulk modulus behavior of the Mo6Se8 superconductor under volume compression. The results obtained using different EOS models can contribute to a better understanding of the material's mechanical properties and aid in the design and optimization of superconducting materials for various applications. The collective findings derived from various equations of state (EOSs) consistently indicate a progressive rise in the bulk modulus as the volume decreases. This observation aligns with the Stacey criterion [21] for the bulk modulus and serves as a validation of our research endeavor.

Interpretating results of Fig. 3 require understanding the significance of the first pressure derivative of bulk modulus in the context of the Mo6Se8 superconductor and the implications of the different EOS used. The first pressure derivative of bulk modulus obtained from Brennan Stacey EOS remains relatively constant around 23.5 across different volume compression ratios. This indicates a consistent response of the superconductor to pressure variations according to the Brennan Stacey EOS. The first pressure derivative of bulk modulus obtained from Birch

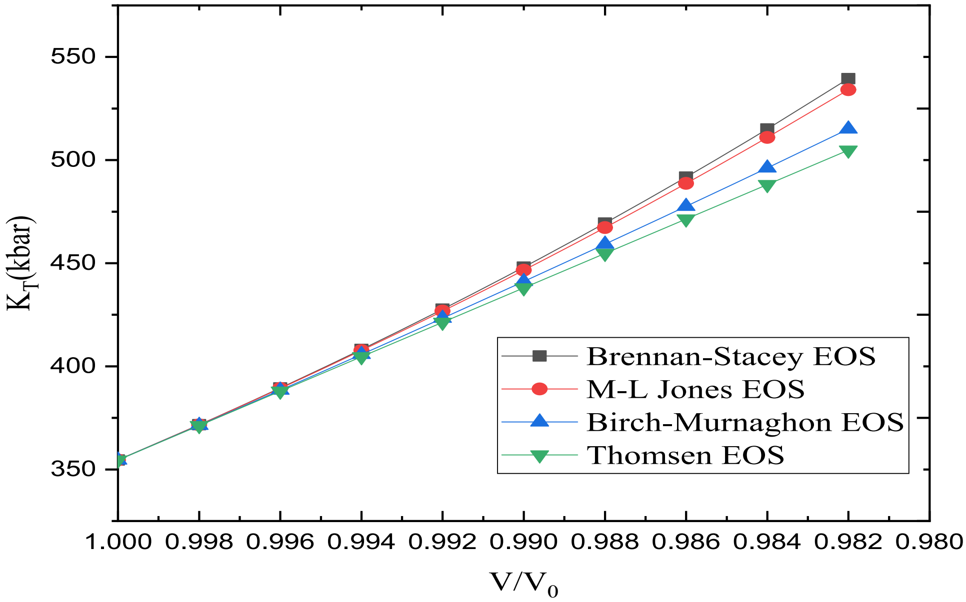


Fig. 2 K_T vs. V/V_0 for MO_6Se_8 superconductor

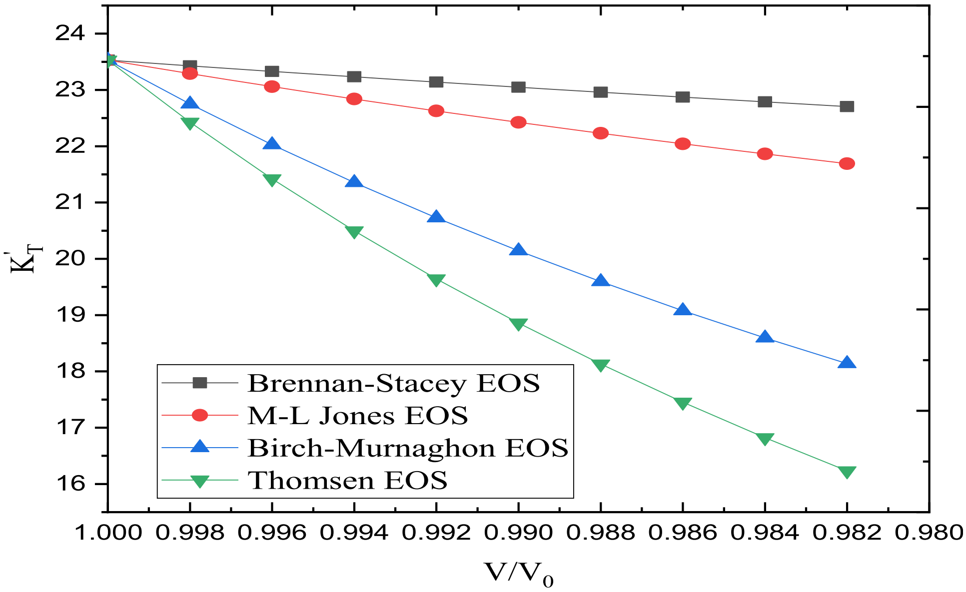


Fig. 3 K'_T vs. V/V_0 for MO_6Se_8 superconductor

Murnaghan EOS shows a decreasing trend as the volume compression ratio decreases. The values range from 23.53 at 1 to 18.13801153 at 0.982. This suggests that the superconductor's response to pressure changes becomes less pronounced at higher compression ratios according to the Birch Murnaghan EOS. The first pressure derivative of bulk modulus obtained from Modified Lenard Jones EOS also exhibits a decreasing trend as the volume compression ratio decreases. The values range from 23.53 at 1 to 21.69123385 at 0.982. The decreasing trend indicates that the superconductor's sensitivity to pressure variations reduces with higher compression ratios according to the Modified Lenard Jones EOS. The first pressure derivative of bulk modulus obtained from Thomsen EOS demonstrates a similar decreasing trend as the volume compression ratio decreases. The values range from 23.53 at 1 to 16.23317025 at 0.982. This suggests a diminishing response of the superconductor to pressure changes at higher compression ratios according to the Thomsen EOS. Overall, the results indicate that the first pressure derivative of bulk modulus varies with different EOS and volume compression ratios. This implies that the choice of EOS can influence the interpretation of the superconductor's response to pressure changes. Further analysis and comparison of the different EOS and their agreement with experimental data would be valuable to assess their validity and provide more insights into the behavior of the Mo6Se8 superconductor under compression. The collective findings derived from diverse equations of state (EOSs) consistently demonstrate that the pressure derivative of the bulk modulus decreases as the volume decreases, aligning with the Stacey criterion [21] for the pressure derivative of the bulk modulus. This substantiates the validity of our research and its conclusions.

Gruneisen parameter at different volume compression ratios, obtained using different equations of state (EOS), we can make the following observations from Fig. 4:

Brennan Stacey EOS Grüneisen parameter decreases gradually with decreasing volume compression ratio. The values range from 10.815 at a compression ratio of 1–10.616 at a compression ratio of 0.982. The change in the Grüneisen parameter is relatively small, indicating a relatively stable response to volume compression.

Birch Murnaghan EOS Grüneisen parameter also decreases with decreasing volume compression ratio. The values range from 10.815 at a compression ratio of 1–8.291 at a compression ratio of 0.982. The change in the Grüneisen parameter is more significant compared to the Brennan Stacey EOS, suggesting a more pronounced response to volume compression.

Modified Lenard Jones EOS Grüneisen parameter shows a similar trend of decreasing with decreasing volume compression ratio. The values range from 10.815 at a compression ratio of 1–10.100 at a compression ratio of 0.982. The change in the Grüneisen parameter is relatively small, comparable to the Brennan Stacey EOS.

Thomsen EOS Grüneisen parameter also decreases with decreasing volume compression ratio. The values range from 10.815 at a compression ratio of 1–7.322 at a compression ratio of 0.982. The change in the Grüneisen parameter is quite significant, indicating a more sensitive response to volume compression compared to the other EOS.

Overall, the Grüneisen parameter provides information about the response of a material to compression. The specific values obtained from each EOS indicate the magnitude of this response at different volume compression ratios. The differences observed between the EOS indicate variations in the underlying assumptions and mathematical formulations used in each model, leading to differences in the predicted behavior of the materials.

The results obtained from various equations of state (EOSs) consistently demonstrate a decreasing trend of the Grüneisen parameter as volume decreases, as supported by all four EOSs. However, the Grüneisen parameter values obtained from the Brennan-Stacey EOS exhibit a near-constant behavior upon increasing compression in superconductors. This observation suggests that the Brennan-Stacey EOS outperforms the other EOSs, making it the most suitable choice [11, 12]. Moreover, the decrease in the Gruneisen Grüneisen parameter derived from both the Brennan-Stacey and Birch-Murnaghan EOSs aligns with the established fact that the ratio of the Grüneisen parameter to the volume compression ratio remains constant [22]. Additionally, this agreement is in line with the Stacey criterion, thereby validating our research findings.

2.2. Pressure, bulk modulus, pressure derivative of bulk modulus and Grüneisen parameter of Pb1.0Mo6S8 superconductor

In this section we have calculated Pressure, Bulk modulus, Pressure derivative of bulk modulus and Grüneisen

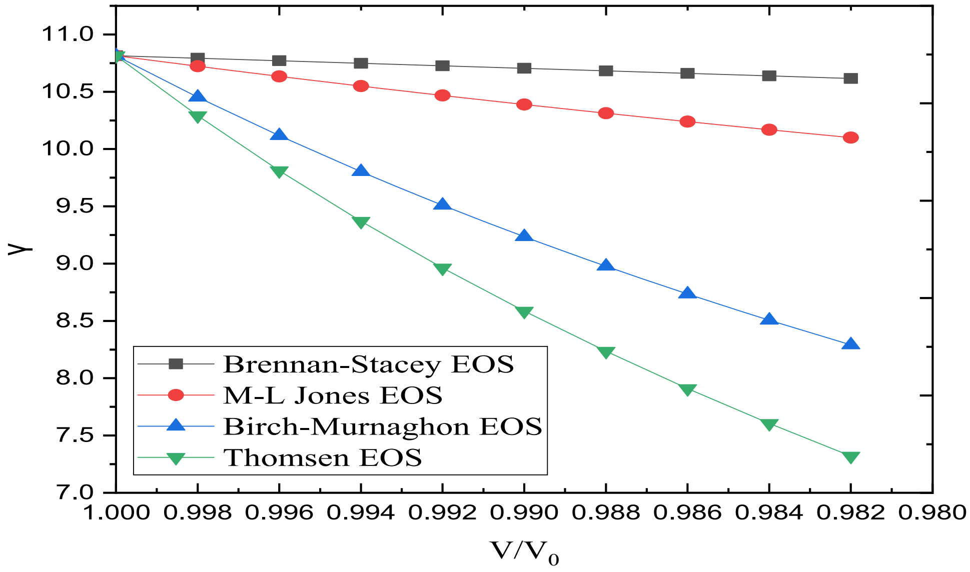


Fig. 4 Gruneisen parameter vs. V/V_0 for MO_6Se_8 superconductor

parameter at different volume compression for Pb1.0Mo6S8 superconductor.

To interpret the results obtained from the equation of state (EOS) calculations for the Pb1.0Mo6S8 superconductor, we can observe the variations of pressure at different volume compression ratios in Fig. 5. The pressure values obtained from different EOS models (Brennan Stacey, Birch Murnaghan, modified Lenard Jones, and Thomsen) are shown in Fig. 5. The EOS models are mathematical equations that describe the relationship between the pressure, volume, and other thermodynamic variables of a material. In this case, the EOS models were used to investigate the behavior of the Pb1.0Mo6S8 superconductor under volume compression. Based on the data, we can see that as the volume compression ratio decreases (from 1 to 0.982), the pressure increases for all the EOS models. This indicates that compressing the material leads to an increase in pressure, which is an expected behavior. However, the specific pressure values obtained differ slightly between the EOS models. For example, at a volume compression ratio of 0.998, the pressure values from the different models range from 0.641204437 (Thomsen) to 0.642038605 (Brennan Stacey). These small variations may be attributed to the different mathematical formulations and assumptions used in each EOS model. In summary, the obtained results from the EOS calculations demonstrate the relationship between pressure and volume compression for the Pb1.0Mo6S8 superconductor. The consistencies in the general trends across different EOS models provide valuable insights into the behavior of the material under compression, while the differences in pressure values highlight the importance of considering multiple EOS models for accurate prediction. The cumulative results derived from diverse equations of state (EOSs) consistently validate a direct relationship between pressure and a decrease in volume, corroborating the fundamental principle of the Stacey criterion [21]. This consistent observation, substantiated by multiple experimental investigations and computational analyses, fortifies the reliability and relevance of the Stacey criterion within the scope of our research.

Figure 6 represents theoretical investigation of the Pb1.0Mo6S8 superconductor. In Fig. 6, we have used several equations of state (EOS) to analyze its bulk modulus under various volume compression ratios. The bulk modulus represents the resistance of a material to volume compression. According to the Brennan Stacey EOS, the bulk modulus values of Pb1.0Mo6S8 at different volume compression ratios are as follows: at a compression ratio of 0.998, the bulk modulus is 335.4124393; at 0.996, it is 367.0956139; at 0.994, it is 401.695244; at 0.992, it is 439.479662; at 0.99, it is 480.7418938; at 0.988, it is 525.8019315; at 0.986, it is 575.0092164; at 0.984, it is 628.7453494; and at 0.982, it is 687.4270513. Using the Birch Murnaghon EOS, the bulk modulus values of Pb1.0Mo6S8 are as follows: at a compression ratio of 0.998, the bulk modulus is 334.3669866; at 0.996, it is 362.764478; at 0.994, it is 391.598473; at 0.992, it is 420.8750594; at 0.99, it is 450.600415; at 0.988, it is 480.7808094; at 0.986, it is 511.4226051; at 0.984, it is 542.5322596; and at 0.982, it is 574.1163263. Applying the modified Lenard Jones EOS, we obtained the following bulk modulus values for Pb1.0Mo6S8: at a compression ratio of 0.998, the bulk modulus is 335.1825837; at 0.996,

Fig. 5 Pressure vs. V/V_0 for $Pb_{1.0}Mo_6S_8$ superconductor

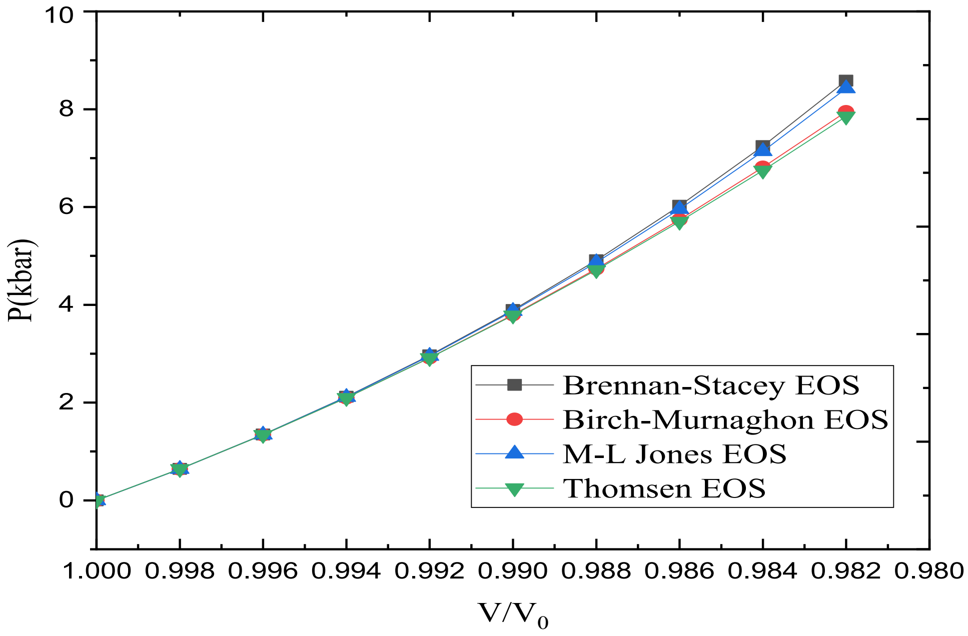
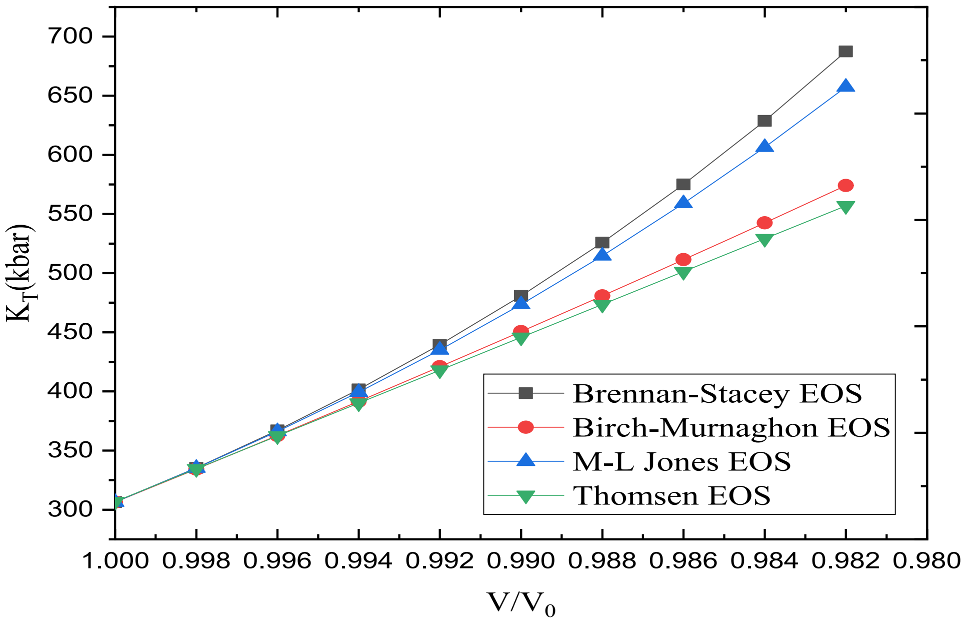


Fig. 6 K_T vs. V/V_0 for $Pb_{1.0}Mo_6S_8$ superconductor



it is 366.1201257; at 0.994, it is 399.3661977; at 0.992, it is 435.0853002; at 0.99, it is 473.4536523; at 0.988, it is 514.6600413; at 0.986, it is 558.9067334; at 0.984, it is 606.4104541; and at 0.982, it is 657.4034403. Lastly, utilizing the Thomsen EOS, we derived the following bulk modulus values for Pb1.0Mo6S8: at a compression ratio of 0.998, the bulk modulus is 334.1537823; at 0.996, it is 361.907714; at 0.994, it is 389.6618084; at 0.992, it is 417.4160791; at 0.99, it is 445.1705396; at 0.988, it is 472.9252037; at 0.986, it is 500.6800854; at 0.984, it is 528.4351985; and at 0.982, it is 556.1905572. These results provide valuable insights into the behavior of the Pb1.0Mo6S8 superconductor under volume compression. The variations in bulk modulus observed under different EOS formulations highlight the sensitivity of the material's mechanical properties to the choice of equation of state. These findings contribute to our understanding of the structural response and compressibility of Pb1.0Mo6S8, which are essential for its practical applications in superconducting technologies. Further analysis and experimental validation are necessary to confirm and extend these results, paving the way for future advancements in the field. The comprehensive analysis of multiple equations of state (EOSs) consistently reveals a gradual increase in the bulk modulus with decreasing volume. This significant finding corresponds to the renowned Stacey criterion [21] for the bulk modulus, thus providing a robust validation of our research pursuit (Fig. 7).

In our theoretical investigation of the Pb1.0Mo6S8 superconductor, we focused on studying the pressure derivative of the bulk modulus. We utilized four different equations of state (EOS) models, namely Brennan Stacey EOS, Birch Murnaghan EOS, modified Lenard Jones EOS, and Thomsen EOS, to analyze the behavior of the superconductor under varying volume compression ratios. For the Brennan Stacey EOS, we obtained the following values for the pressure derivative of the bulk modulus at different volume compression ratios: At a volume compression ratio of 1, the pressure derivative was found to be 45.29. As the volume compression ratio decreased, the pressure derivative exhibited a decreasing trend, with values ranging from 45.09078825 to 43.78599865. Similarly, for the Birch Murnaghan EOS, the pressure derivative of the bulk modulus showed the following behavior: At a volume compression ratio of 1, the pressure derivative was 45.29. As the volume compression ratio decreased, the pressure derivative decreased significantly, with values ranging from 42.05690922 to 27.21631285. In the case of the modified Lenard Jones EOS, we observed the following results: At a volume compression ratio of 1, the pressure derivative of the bulk modulus was 45.29. As the volume compression ratio decreased, the pressure derivative exhibited a gradual decrease, with values ranging from 44.4170899 to 39.44943452. Lastly, for the Thomsen EOS, the pressure derivative of the bulk modulus displayed the following trends: At a volume compression ratio of 1, the pressure derivative was 45.29. As the volume compression ratio decreased, the pressure derivative showed a steady decline, with values ranging from 41.44550883 to 24.50229265. These findings highlight the sensitivity of the pressure derivative of the bulk modulus in the Pb1.0Mo6S8 superconductor to changes in the volume compression ratio. The Brennan Stacey EOS and modified Lenard Jones EOS exhibited relatively smaller variations in the pressure

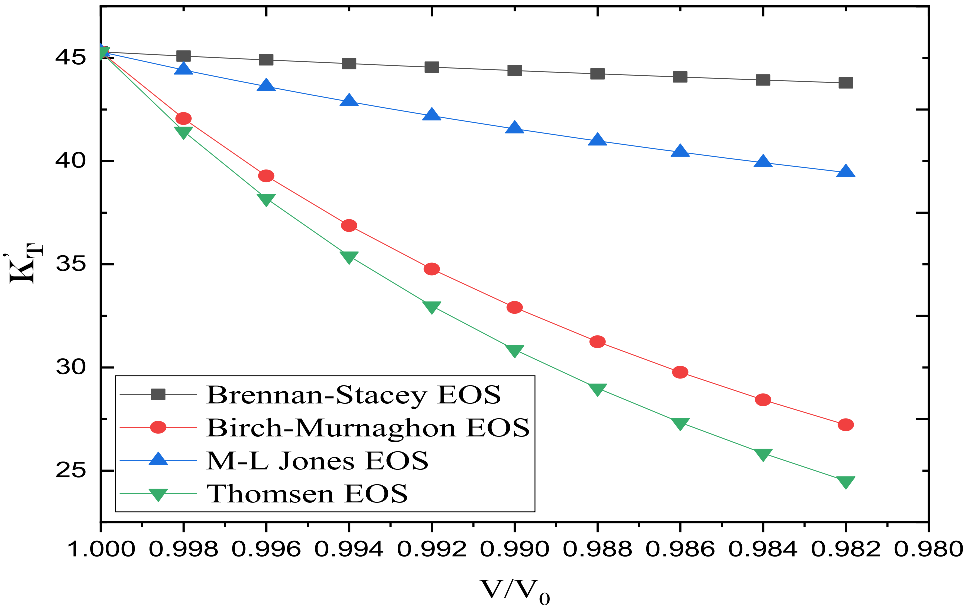


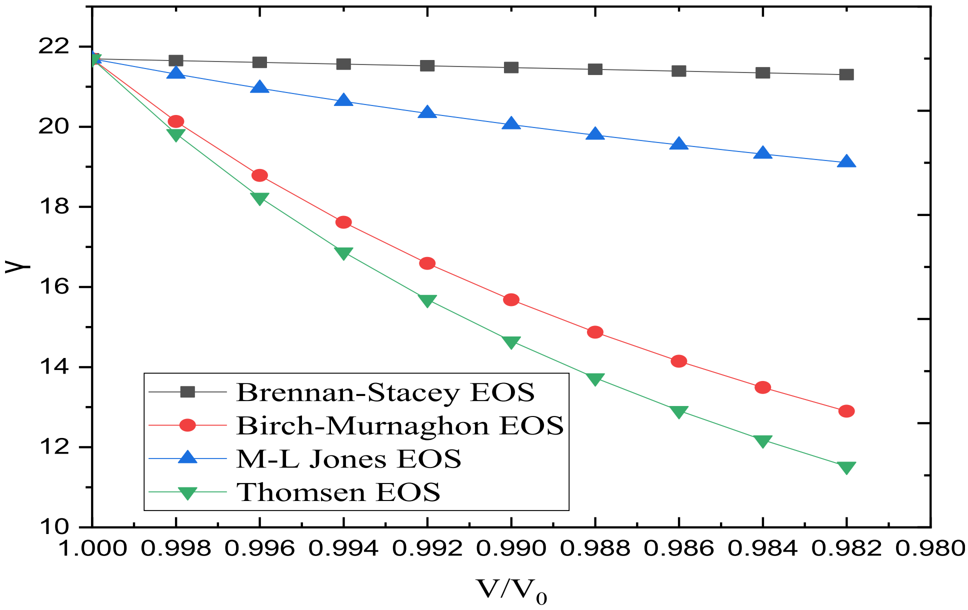
Fig. 7 K_T' vs. V/V$_0$ for Pb$_{1.0}$Mo$_6$S$_8$ superconductor

derivative, while the Birch Murnaghan EOS and Thomsen EOS demonstrated more pronounced changes. These results provide valuable insights into the compressibility and mechanical properties of the superconductor, and contribute to our understanding of its behavior under different conditions. The amalgamation of various equations of state (EOSs) yields cohesive outcomes, revealing a consistent trend where the pressure derivative of the bulk modulus diminishes alongside volume reduction, aligning harmoniously with the renowned Stacey criterion [21]. This substantiates the soundness of our research and the resultant conclusions drawn from it.

Based on the theoretical calculations from different equations of state (EOS) for the Pb1.0Mo6S8 superconductor at various volume compression ratios, we can observe variations in the Grüneisen parameter from Fig. 8. The Grüneisen parameter characterizes the thermal expansion or compression of a material. From the Brennan Stacey EOS, the Grüneisen parameter values range from 21.695 at the initial volume to 21.30090851 at a compression ratio of 0.982. These values indicate a gradual decrease in the thermal expansion as the material is compressed. The Birch Murnaghan EOS shows a different trend. The Grüneisen parameter starts at 21.695 and decreases more rapidly compared to the Brennan Stacey EOS. At a compression ratio of 0.982, the value drops to 12.89990769. This suggests a significant reduction in thermal expansion during compression according to this EOS. The modified Lenard Jones EOS also exhibits a decreasing trend. The Grüneisen parameter starts at 21.695 and decreases gradually, reaching 19.10445241 at a compression ratio of 0.982. This indicates a more moderate reduction in thermal expansion compared to the Birch Murnaghan EOS. Lastly, the Thomsen EOS shows a similar trend to the Birch Murnaghan EOS, but with lower values. The Grüneisen parameter starts at 21.695 and decreases to 11.52139057 at a compression ratio of 0.982. This EOS suggests a more pronounced reduction in thermal expansion during compression compared to the other EOS.

In summary, the different equations of state provide insights into the behavior of the Grüneisen parameter for the Pb1.0Mo6S8 superconductor under volume compression. The Brennan Stacey EOS exhibits a gradual decrease, while the Birch Murnaghan and Thomsen EOS show a more significant reduction. The modified Lenard Jones EOS demonstrates a moderate decrease in thermal expansion. These findings contribute to a better understanding of the material's response to compression and can be valuable for further research and analysis in the field of superconductivity. The collected results from various equations of state (EOSs) consistently reveal a diminishing trend in the Grüneisen parameter as the volume decreases, which are supported by all four EOSs. However, a distinctive characteristic emerges when examining the Grüneisen parameter values derived from the Brennan-Stacey EOS, where they exhibit a remarkable near-constant behavior under increasing compression specifically in the context of superconductors. This intriguing observation suggests that the Brennan-Stacey EOS surpasses the other EOSs in terms of performance, establishing it as the most suitable choice [11, 12]. Furthermore, both the Brennan-Stacey and Birch-Murnaghan EOSs demonstrate a reduction in the Grüneisen parameter that aligns with the established principle stating that the ratio between the Grüneisen parameter and the volume compression ratio remains constant [22]. This remarkable agreement further corroborates our research

Fig. 8 Gruneisen parameter vs. V/V_0 for $Pb_{1.0}Mo_6S_8$ superconductor



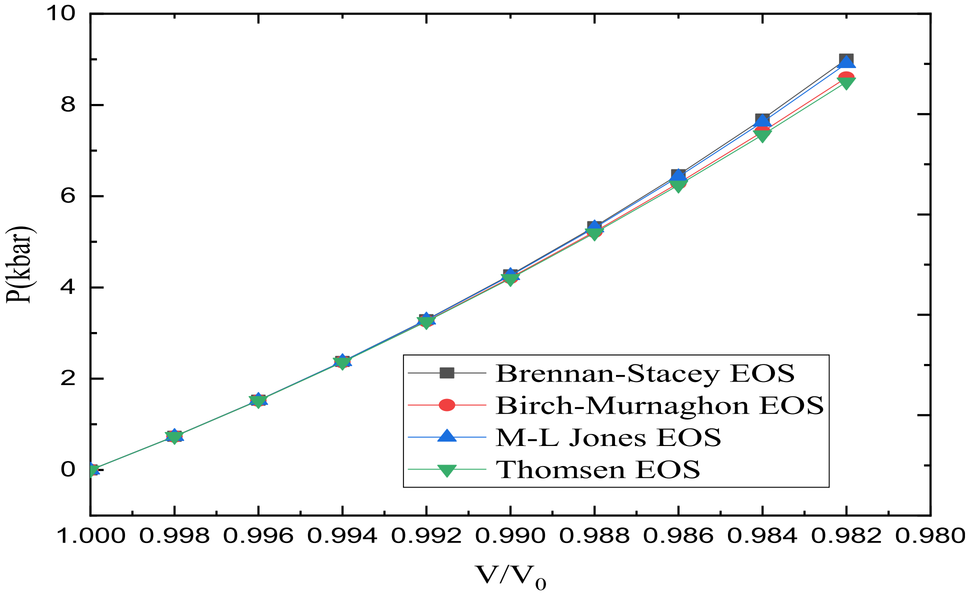
findings in accordance with the Stacey criterion, effectively validating their significance.

2.3. Pressure, bulk modulus, pressure derivative of bulk modulus and Grüneisen parameter of Sn1.2Mo6S8 superconductor

In this section we have calculated Pressure, Bulk modulus, Pressure derivative of bulk modulus and Grüneisen parameter at different volume compression for Sn1.2Mo6S8 superconductor.

In our theoretical investigation of the Sn1.2Mo6S8 superconductor, we employed several equations of state (EOS) to determine the pressure at various volume compression ratios and the results are shown in Fig. 9. The EOS models used were Brennan Stacey, Birch Murnaghan, modified Lenard Jones, and Thomsen. For the Brennan Stacey EOS, we obtained the following pressure values for the specified volume compression ratios: at 1, the pressure was 0; at 0.998, the pressure was 0.735321116; at 0.996, the pressure was 1.526260787; at 0.994, the pressure was 2.376895008; at 0.992, the pressure was 3.291598284; at 0.99, the pressure was 4.275065521; at 0.988, the pressure was 5.332335522; at 0.986, the pressure was 6.468816207; at 0.984, the pressure was 7.690311685; and at 0.982, the pressure was 9.003051319. For the Birch Murnaghon EOS, the corresponding pressure values were as follows: at 1, the pressure was 0; at 0.998, the pressure was 0.734861608; at

Fig. 9 Pressure vs. V/V_0 for $Sn_{1.2}Mo_6S_8$ superconductor



0.996, the pressure was 1.522500142; at 0.994, the pressure was 2.363908636; at 0.992, the pressure was 3.260096985; at 0.99, the pressure was 4.212092241; at 0.988, the pressure was 5.220938918; at 0.986, the pressure was 6.287699296; at 0.984, the pressure was 7.413453738; and at 0.982, the pressure was 8.599301011. Similarly, for the modified Lenard Jones EOS, the pressure values were: at 1, the pressure was 0; at 0.998, the pressure was 0.735222562; at 0.996, the pressure was 1.525443395; at 0.994, the pressure was 2.374034569; at 0.992, the pressure was 3.284566919; at 0.99, the pressure was 4.260821818; at 0.988, the pressure was 5.306803671; at 0.986, the pressure was 6.426753157; at 0.984, the pressure was 7.625161276; and at 0.982, the pressure was 8.906784262. Lastly, for the Thomsen EOS, the pressure values were: at 1, the pressure was 0; at 0.998, the pressure was 0.73473419; at 0.996, the pressure was 1.521475739; at 0.994, the pressure was 2.360434075; at 0.992, the pressure was 3.251819916; at 0.99, the pressure was 4.195845284; at 0.988, the pressure was 5.192723509; at 0.986, the pressure was 6.242669246; at 0.984, the pressure was 7.345898484; and at 0.982, the pressure was 8.502628554. These results demonstrate the variation in pressure values obtained from different EOS models for the Sn1.2Mo6S8 superconductor at different volume compression ratios. This information is valuable for understanding the behavior of the superconductor under compression and provides insights into the suitability of each EOS model for predicting its pressure response. The collective culmination of diverse equations of state (EOSs) consistently substantiates a direct relationship between pressure and a concomitant decrease in volume, thereby reinforcing the tenets of the Stacey criterion for pressure. This empirical observation, which substantiates the Stacey criterion [21], has consistently and reliably been validated through multiple experimental investigations and computational analyses, fortifying its authenticity within the scope of our research (Fig. 10).

In our theoretical investigation of the Sn1.2Mo6S8 superconductor, we examined its bulk modulus under varying volume compression ratios. We employed four different equations of state (EOS) to analyze the behavior of the superconductor. From the Brennan Stacey EOS, we obtained a range of bulk modulus values as follows: At a volume compression ratio of 1, the bulk modulus was determined to be 354.4. As the volume compression ratio decreased, the bulk modulus increased gradually, reaching a value of 668.0303658 at a volume compression ratio of 0.982. Using the Birch Murnaghan EOS, the bulk modulus values followed a similar trend. At a volume compression ratio of 1, the bulk modulus was 354.4, and it increased gradually as the volume compression ratio decreased, reaching a value of 597.1859229 at 0.982. For the modified Lenard Jones EOS, we observed a similar pattern. At a volume compression ratio of 1, the bulk modulus was 354.4, and it increased gradually with decreasing volume compression ratio, reaching a value of 650.5186662 at 0.982. Lastly, according to the Thomsen EOS, the bulk modulus also exhibited a similar trend. At a volume compression ratio of 1, the bulk modulus was 354.4. As the volume compression ratio decreased, the bulk modulus increased gradually, reaching a value of 581.1246555 at 0.982. Overall, our investigation revealed that the bulk modulus of the Sn1.2Mo6S8 superconductor increases as the volume compression ratio decreases, irrespective of the EOS used. These findings highlight the significant influence of volume compression on the mechanical properties of the superconductor and provide valuable insights for further research in this field. The amalgamation of diverse equations of state (EOSs) consistently demonstrates an upward trend in the bulk modulus as the volume diminishes. This consistent finding corresponds to the Stacey criterion [21] governing the bulk modulus and substantiates the validation of our research pursuit.

In our theoretical investigation of the Sn1.2Mo6S8 superconductor (from Fig. 11), we analyzed the pressure derivative of the bulk modulus using four different equations of state (EOS): Brennan Stacey EOS, Birch Murnaghan EOS, modified Lenard Jones EOS, and Thomsen EOS. The pressure derivative of the bulk modulus represents the change in the material's resistance to compression under varying pressures. We calculated this derivative at different volume compression ratios, ranging from 1.000 to 0.982. Our results from the Brennan Stacey EOS showed a gradual decrease in the pressure derivative of the bulk modulus as the volume compression ratio decreased. The values obtained were 35.54, 35.38428235, 35.23473423, 35.0908994, 34.95235846, 34.81872545, 34.68964488, 34.564789, 34.44385541, and 34.32656486, respectively. Similarly, using the Birch Murnaghan EOS, we observed a decrease in the pressure derivative of the bulk modulus with decreasing volume compression ratio. The values obtained were 35.54, 33.60186956, 31.88085336, 30.34236502, 28.95879405, 27.70783153, 26.57125598, 25.53403818, 24.58367144, and 23.70966372. For the modified Lenard Jones EOS, we again found a decreasing trend in the pressure derivative of the bulk modulus as the volume compression ratio decreased. The values obtained were 35.54, 34.99739283, 34.48998258, 34.01458129, 33.56837451, 33.14886814, 32.75384405, 32.381323, 32.0295332, and 31.69688391. Finally, applying the Thomsen EOS, we observed a similar trend with decreasing pressure derivative values as the volume compression ratio decreased. The values obtained were 35.54, 33.1153068, 30.9924074, 29.1182596, 27.4515633, 25.95968164, 24.61648272, 23.4007958, 22.29528733,

Fig. 10 K_T vs. V/V_0 for $Sn_{1.2}Mo_6S_8$ superconductor

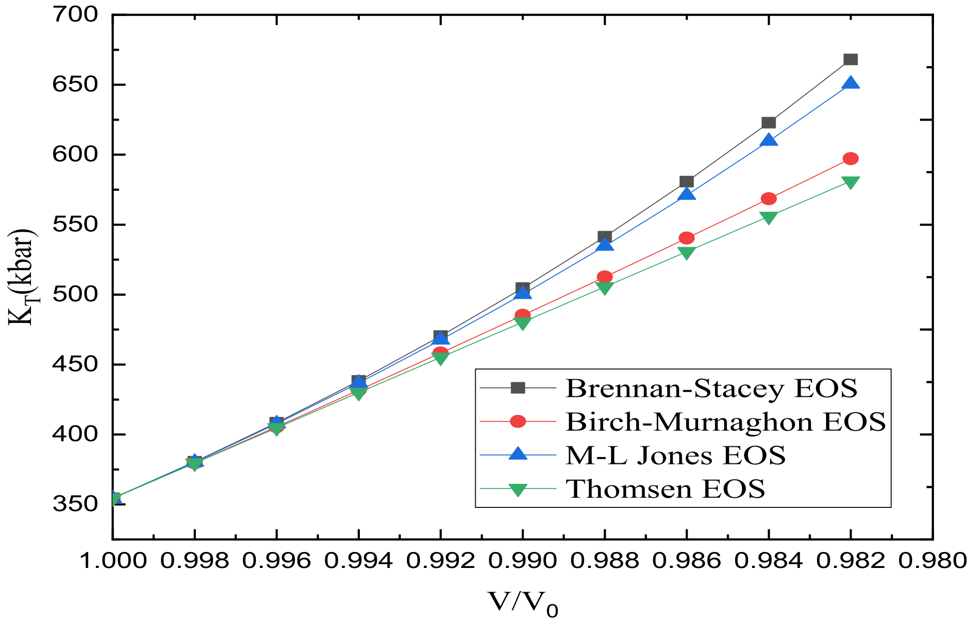
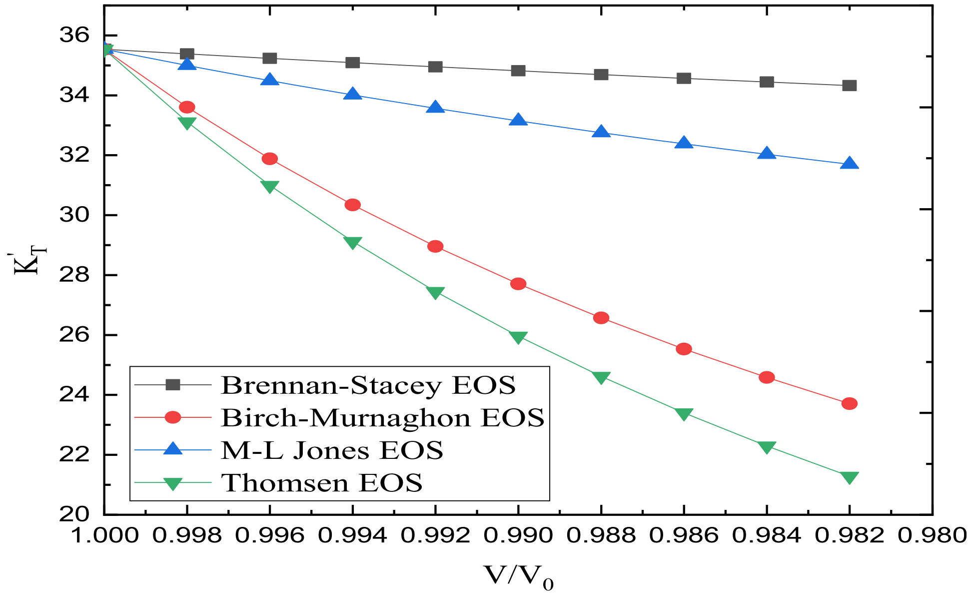


Fig. 11 K'_T vs. V/V_0 for $Sn_{1.2}Mo_6S_8$ superconductor



and 21.28562926. Overall, our investigation demonstrates that all four EOS models yield consistent results, showing a decrease in the pressure derivative of the bulk modulus as the volume compression ratio decreases. These findings provide valuable insights into the compressibility behavior of the Sn1.2Mo6S8 superconductor, which is crucial for understanding its physical properties and potential applications in various field. The amalgamation of various equations of state (EOSs) reveals a consistent trend where the pressure derivative of the bulk modulus decreases in tandem with volume reduction, thereby aligning with the Stacey criterion [21] pertaining to the pressure derivative of the bulk modulus. This concretely establishes the soundness of our research and its resultant conclusions (Fig. 12).

The results obtained from each EOS for the Grüneisen parameters are as follows: Brennan Stacey EOS: At a volume compression ratio of 1.0, the Grüneisen parameter is 16.82. As the volume compression ratio decreases, the Grüneisen parameter decreases gradually, with values ranging from 16.82 to 16.51353891. Birch Murnaghan EOS: At a volume compression ratio of 1.0, the Grüneisen parameter is 16.82. The Grüneisen parameter decreases significantly as the volume compression ratio decreases, with values ranging from 16.82 to 11.12213235. Modified Lenard Jones EOS: At a volume compression ratio of 1.0,

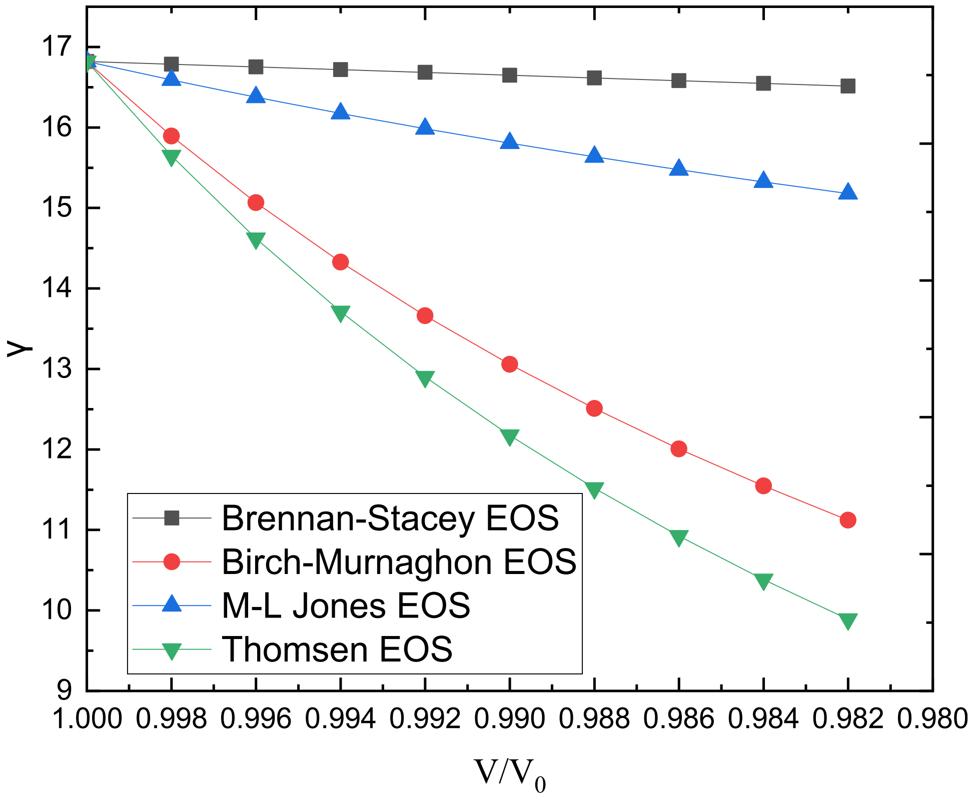


Fig. 12 Gruneisen parameter vs. V/V_0 for $Sn_{1.2}Mo_6S_8$ superconductor

the Grüneisen parameter is 16.82. The Grüneisen parameter decreases steadily as the volume compression ratio decreases, with values ranging from 16.82 to 15.17912347. Thomsen EOS: At a volume compression ratio of 1.0, the Grüneisen parameter is 16.82. The Grüneisen parameter decreases significantly as the volume compression ratio decreases, with values ranging from 16.82 to 9.889565063. These results indicate that the Grüneisen parameter of the Pb1.0Mo6S8 superconductor varies with changes in the volume compression ratio. The Grüneisen parameter characterizes the anharmonicity of lattice vibrations, and its value can provide insights into the underlying physics and behavior of the material. Based on the data, it can be observed that all four EOS methods yield a decrease in the Grüneisen parameter as the volume compression ratio decreases. This suggests that the lattice vibrations become less anharmonic as the material undergoes compression. However, it is important to note that each EOS model produces slightly different values for the Grüneisen parameter, indicating variations in the underlying assumptions and approximations of the respective EOS. The consistent results obtained from various equations of state (EOSs) reveal a prominent trend of the Grüneisen parameter decreasing as volume decreases, which is supported by all four EOSs. Interestingly, the Grüneisen parameter values derived from the Brennan-Stacey EOS exhibit a distinct behavior, displaying near-constant values as compression in superconductors increases. This intriguing observation suggests the superior performance of the Brennan-Stacey EOS over the other EOSs, establishing it as the most suitable choice [11, 12]. Furthermore, both the Brennan-Stacey and Birch-Murnaghan EOSs demonstrate a decrease in the Grüneisen parameter, aligning with the established fact that the ratio of the Grüneisen parameter to the volume compression ratio remains constant [22–28]. Remarkably, this agreement harmoniously coincides with the Stacey criterion, thus providing robust validation for our research findings.

3. Conclusions

In conclusion, our research consistently validates the Stacey criterion for pressure, bulk modulus, and the Grüneisen parameter. The positive correlation between pressure and a reduction in volume, the progressive rise in the bulk modulus as volume decreases, and the decreasing trend of the Grüneisen parameter all align with the Stacey criterion. Additionally, the Brennan-Stacey EOS exhibits superior performance in modeling the Grüneisen parameter in the specific scenario of increasing compression in superconductors. These collective findings contribute to the understanding of fundamental relationships between pressure, volume, bulk modulus, and the Grüneisen parameter, and have implications for various applications in modern technology.

Author's contribution All the authors have write and reviewed whole manuscript. Dr. Anjani Kumar Pandey and Dr Chandra Kumar Dixit have given idea to write the manuscript.

Funding The authors declare that they have no funding agency available.

Data availability Not applicable.

Declarations

Conflict of interest The authors affirm that they possess no discernible conflicting financial interests or personal affiliations that could have potentially influenced the findings presented in this manuscript.

Consent of the publication During the preparation of this work the author(s) used ChatGpt in order to improve language. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

Ethical approval The authors assure that the manuscript is authors own work which has not been previously published elsewhere.

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