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Study Of The Compression Behaviour Of Fe Cr Ti Sn And Fe Cr Ti Sb Materials Using Various Equation Of States

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Abstract

The Heusler compounds assert potential candidates for a variety of applications such as memory devices, spintronics, magneto resistive materials, and spin-value generators owing to their undeniable properties such as large magnetic moment, large ferromagnetism, Curie temperature, high polarization at the Fermi level, thermoelectric performance, etc. In this work, the theoretical approach wherein various equation of states such as Tait, Murnaghan, Shanker, Kohliya and Chandra have been employedto investigate thecompression behaviour of the two Heusler compounds FeCrTiSn and FeCrTiSb in detail. It has been observed that both the compounds FeCrTiSn and FeCrTiSb exhibit a nearly linearly declining trend with the applied pressure and our theoretical results are in agreement with experimental calculated one reported in the literature.

Key words: Magnetic, Thermoelectric, Superconductivity, Materials, Equation of State.

1. Introduction

Electronic and magnetic materials have subsequent applications in different fields [1-5]. Electronic materials have vast applications in the semiconductor industry, particularly in mobile phones, integrated circuits, and electronic chips [6-8]. For instance, silicon has found its way into modern computers, digital timepieces, communication satellites, and pocket calculators. Additionally, magnetic materials are used in devices including magnets, generators, magnetic detectors, microphones, and magnetic separators [9-12]. On the scale of these applications, we considered the class of materials known as “Heusler compounds”.

"Heusler compounds" refers to a class of intermetallic compounds with a definite crystal structure and composition. Heusler compounds classically consist of three elements: two transition metals (one from group VIII and the other from groups III-VI) and a main-group element (e.g., tin, antimony, or arsenic) [13-14]. The general formula for Heusler compounds is X2YZ, where X and Y are transition metals and Z is a main-group element. These compounds have attracted significant interest due to their diverse and unique properties. They exhibit a wide range of electronic, magnetic, and thermal properties, making them useful in various applications such as spintronics, magneto-electronics, thermoelectrics, and catalysis.Some of the major technological applications of such compounds namely FeCrTiSn and FeCrTiSb.

Spintronics: Heusler compounds are used in spintronic devices, which utilize the spin of electrons in addition to their charge. These compounds exhibit high spin polarization and can be used in spin valves, magnetic tunnel junctions, and spin injectors for efficient spin transport and manipulation [15-16].

1. Magnetic materials: Many Heusler compounds exhibit ferromagnetic or ferrimagnetic properties, making them useful in the development of high-performance permanent magnets, magnetic sensors, and magnetic recording.
2. Thermoelectrics: Certain possess a combination of high electrical conductivity and low thermal conductivity, making them promising candidates for thermoelectric applications. These materials can efficiently convert waste heat into electrical energy or be used in solid-state cooling devices.
3. Superconductivity: Some Heusler compounds exhibit superconducting behavior at low temperatures. These materials are being explored for their potential use in high-temperature superconductors and related applications.
4. Energy Storage devices: All under study Heusler compounds exhibit good electrochemical performance, making them potential materials for use in energy storage devices such as batteries

   Because of extraordinary thermal stability, these compounds are appropriate for high-temperature applications.

In this paper, we have calculated the compressional behaviour of Fe based Heusler compounds in terms of calculated values of relative change in volume (V/V_o) and bulk modulus as a function of pressure at constant temperature by using some theoretical models, known as equations of state.

Equation of state is a relationship that designates the state of a system in terms of its variables, such as temperature, pressure, volume, and density [17-26]. It is used to envisage the behaviour of a substance under different conditions viz. pressure, volume and temperature for both systems of a pure component and also for multicomponent mixture. The equations of state are valuable in defining the stability of solid material by varying various parameters like pressure volume entropy and temperature [27-29]. So, the equation of state is a elementary characteristic of a matter which makes promising the application of all the general principles of thermodynamics, and reflects atomic structure, chemical bonding and stability of material [30-32].

2. Methods of Analysis:

In this study, various equations of state (EOS) have been used to determine the compression behaviour of Heusler Febased compounds. Bulk modulus measures the resistance of a material to change in volume when subjected to an external pressure and is determined by the ratio of the infinitesimal change in pressure to the corresponding fractional change in volume. In the present study we have used Tait equation state, Murnaghan EOS, Kohliya and Chandra and Shankers equation of state, to determine the pressure dependence of volume compression and bulk modulus of some Heusler compounds namely FeCrTiSn and FeCrTiSb.

Tait equation of state generally fits finest for the compression behaviour of the chosen material had given by P.G. Tait in 1888, which was the non-linear relation of compression with pressure for liquids. After many modifications the new modified form of equation of state is introduced known as Usual Tait equation (UTE) is in the following form for different solids.

$$\frac{V}{V_0} = \left[1 - \frac{1}{K_0' + 1}\ln\left\{1 + \left(\frac{K_0' + 1}{K_0}\right)P\right\}\right] \text{....(1)}$$

Using this realistic approach we can calculate the relative compression V/V_0 for different solids.

Also, the expression for isothermal bulk modulus K(P)by using equation (3.27) can be written as:

$$K = K_0 \frac{V}{V_0}\left\{1 + \frac{K_0' + 1}{K_0}P\right\} \quad \text{... (2)}$$

From equation (1)

$$1 + \frac{K_0' + 1}{K_0}P = \exp\left\{\left(1 - \frac{V}{V_0}\right)(K_0' + 1)\right\} \quad \text{... (3)}$$

Putting equation (3.29) in equation (3.28) we get

$$K(P) = K_0 \frac{V}{V_0}\exp\left\{(K_0' + 1)\left(1 - \frac{V}{V_0}\right)\right\} \qquad \text{...(4)}$$

Which is the Tiat equation for isothermal bulk modulus.

Other equations of states, Murnaghan equation of state, Kholiya and Chandra equation of state and Shankers equation of state aregiven by the following relations:

Murnaghan EOS [33-34] is given by the relation

$$P = \frac{B_0}{B_0'}\left[\exp\left\{-B_0' \ln\left(\frac{V}{V_0}\right)\right\} - 1\right] \text{....(5)}$$

Kohliya and Chandra [35- 36] equation of state is given the relation

$$P = \frac{B_0}{2}\left[(B_0' - 3) - 2(B_0' - 2)\left(\frac{V}{V_0}\right)^{-1} + (B_0' - 1)\left(\frac{V}{V_0}\right)^{-2}\right] \ldots (6)$$

Shankers equation of state [35-38] is given by the equation

$$P = B_0\left[\left(1 - \frac{V}{V_0}\right) + \left(B_0' + \frac{1}{2}\right)\left(1 - \left(\frac{V}{V_0}\right)^2\right)\right] \ldots (7)$$

3. Results and Discussion:

Table 1: Compression behaviour of **FeCrTiSb** predicted by various EOS

Pressure (GPa)	Tait Equation of State	Murnaghan Equation of State	Kholiya and Chandra Equation of State	Shankers Equation of State
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.991	0.9917	0.9927	0.9938
4	0.9815	0.9819	0.9831	0.9841
6	0.9699	0.971	0.9742	0.9732
8	0.9601	0.9591	0.9613	0.963
10	0.9508	0.9503	0.951	0.952
12	0.9411	0.942	0.9427	0.944
14	0.934	0.933	0.9371	0.9377

Table 1 presents the compression behaviour of **FeCrTiSb** at different pressures (in GPa) as predicted by different equations of state: Tait, Murnaghan, Kholiya and Chandra, and Shankers (shown in Fig 1. The table indicates that as the pressure increases, the volume of FeCrTiSb decreases, which is consistent with the behaviour of most materials under compression. The Tait equation of state predicts a gradual decrease in volume, with a V/V_0 value of 0.934 at 14GPa. The Murnaghan equation of state also predicts a gradual decrease in volume, with a slightly higher V/V_0 value of 0.933 at 14GPa. The Kholiya and Chandra equation of state predicts a slightly more rapid decrease in volume, with a V/V_0 value of 0.9371 at 14 GPa. The Shankers equation of state predicts the most rapid decrease in volume, with a V/V_0 value of 0.9377 at 14 GPa.

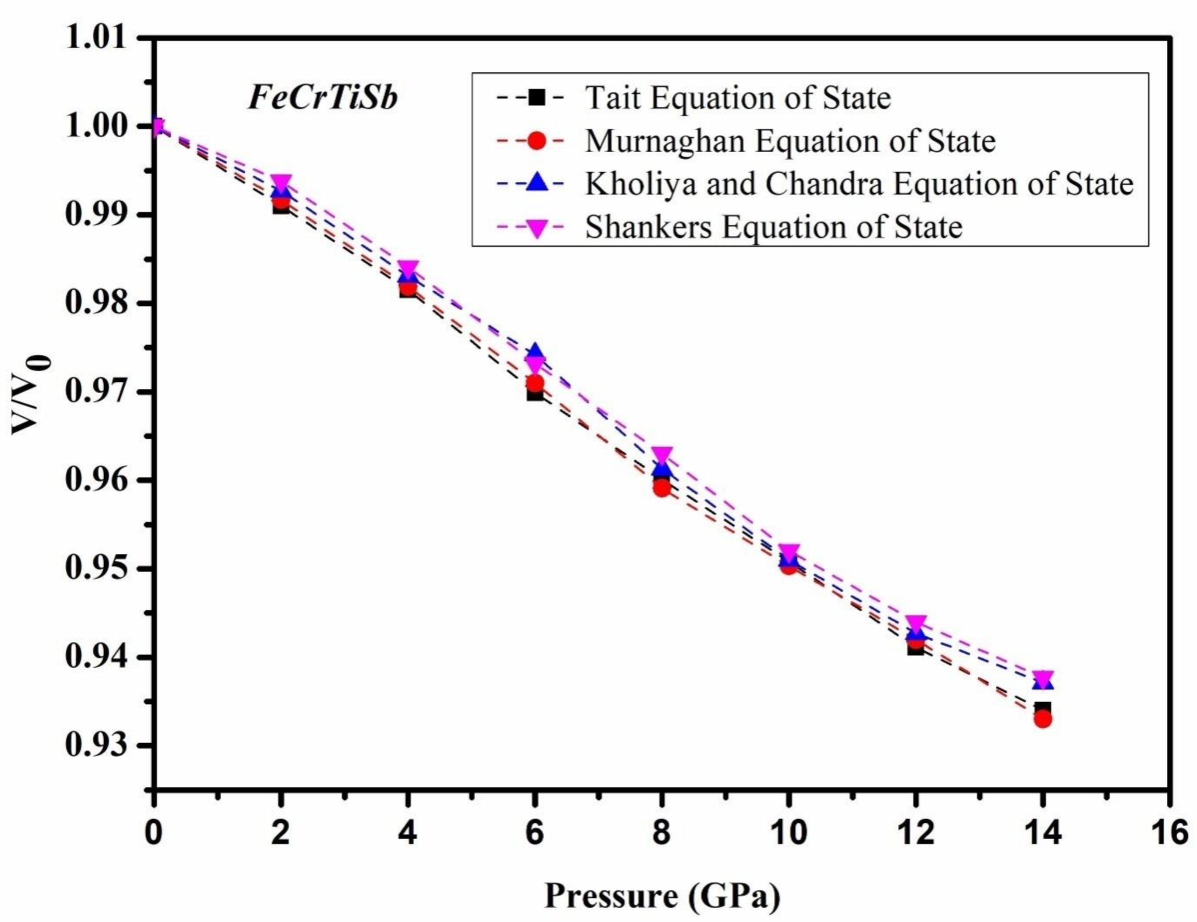

Fig 1. Volume compression with respect to Pressure for **FeCrTiSb**

Table 2: Compression behaviour of **FeCrTiSn** predicted by various EOS

Pressure (GPa)	Tait Equation of State	Murnaghan Equation of State	Kholiya and Chandra Equation of State	Shankers Equation of State
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.9902	0.9912	0.9913	0.9922
4	0.9815	0.9824	0.984	0.9841
6	0.9718	0.9737	0.975	0.975
8	0.9612	0.9633	0.963	0.9646
10	0.951	0.9531	0.9551	0.9565
12	0.943	0.9452	0.946	0.9483

14	0.9361	0.9387	0.9382	0.9388

Table 2 presents the compression behaviour of **FeCrTiSn** at different pressures (in GPa) as predicted by different equations of state: Tait, Murnaghan, Kholiya and Chandra, and Shankers (shown in Fig 2). The table indicates that as the pressure increases, the volume of FeCrTiSn decreases, which is consistent with the behaviour of most materials under compression. The Tait equation of state predicts a gradual decrease in volume, with a V/V_0 value of 0.9361 at 14GPa. The Murnaghan equation of state also predicts a gradual decrease in volume, with a slightly higher V/V_0 value of 0.9387 at 14GPa. The Kholiya and Chandra equation of state predicts a slightly more rapid decrease in volume, with a V/V_0 value of 0.9381 at 14 GPa. The Shankers equation of state predicts the most rapid decrease in volume, with a V/V_0 value of 0.9388 at 14 GPa.

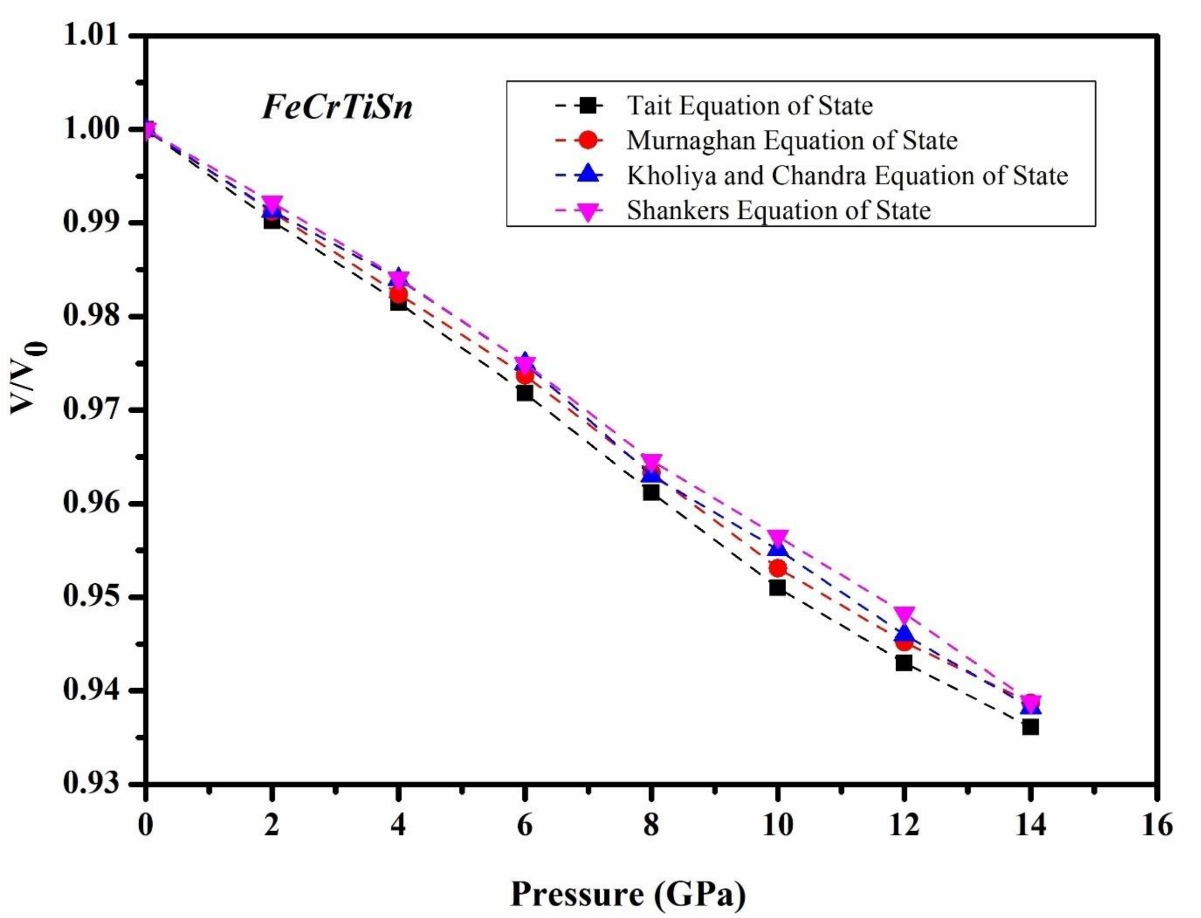

Fig 2. Volume compression with respect to Pressure for **FeCrTiSn**

4. Conclusions:

This study investigated the compression behaviour of FeCrTiSn and FeCrTiSb using Various Equation of Statesin terms of computed values of bulk modulus and relative change in volume (V/V_0) as a function of pressure at constant temperature. The study revealed that the compression behaviour of the materials under study varies with pressure and with the type of equation of state used to fit the data. Further, the Tait equation of state generally fits best for the compression behaviour of the materials, followed by the Murnaghan equation of state, and the Kholiya and Chandra and Shankers equations of state. Boththe Heusler compounds FeCrTiSn and FeCrTiSb show similar patterns in compression behaviour with decreasing volume with increasing pressure. It is evident from the data that the studied materials possess different compressibility due to their unique structural and electronic properties.

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