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Theoretical prediction of equation of state for semiconductors

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Abstract

The isothermal EOS provides a powerful tool for theoretical prediction of different thermo elastic properties at extreme compressions. In the present work an attempt has been made for theoretical computation of pressure dependence of compression for different semi conducting materials viz. $FeSi_2$, SnS, , AlN, GaN, MoN, For this computation four different isothermal EOS viz. Tait EOS , Murnaghan EOS, Shanker EOS, and Suzuki EOS are used . The obtained results are compared with available experimental data which reveals that Murnaghan EOS is best suited for theoretical prediction of compression for semiconductors at different pressure ranges.

Keywords: Semiconductors; Compression; Equation of State.
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1. Introduction

The application of pressure plays a major role in optical investigations of electronic states in the artificial semiconductor structures such as quantum well and super lattices. The high pressure allows for a controlled reduction of interatomic distances and a continuous modification of the chemical bonding. On the other hand, the interatomic distances are also the input parameter in most theoretical model of solid state properties. For this reason there exists a closed link between theory and high pressure experiments in general.

The semiconducting materials have intermediate electrical properties lies between conductor and insulators which are determined by crystal structure and electronic energy bands. A lot of work has been done in the area of their electrical and structural properties [1-6] but not well understood about the thermo physical properties of these materials. The modern technology is also based on the semiconductor devices so there is a need of EOS which can describe the compressional behavior of semiconductors under extreme compression ranges.

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The recent progress made on the synthesis of porous materials *via* SCS is also capable of growing metal oxide thin films at low temperatures, enabling the fabrication of low-cost and high-performance electronics on flexible plastic substrates [7]. Reshak and Jamal have searched 1D and 2D EOS for MnAs and Mg within PBE functional and compared the results with experimental data, the results of 2D search for EOS are better than 1D search of EOS which are very useful to estimate exact elastic properties of the materials at extreme physical conditions [8]. Molecular-dynamics simulation with the three-body potential of Tersoff is an extremely powerful technique, suggesting that its extension to more complicated structures like the ternary or quaternary semiconductors alloys and metastable alloys will produce satisfactory results as well [9].

The Equation of state (EOS) is a fundamental relation between pressure, temperature and volume to analyze the thermo elastic properties of solids. The iron disilicide (FeSi2) is an important semiconductor because of its wide use in optical fiber communications [10]. This material is also known as ecologically friendly semiconductor [1,2]. The tin sulphide (SnS) is an important material for optoelectronics devices. SnS undergoes a phase transition from orthorhombic to monoclinic at 18.15 GPa. MoN is member of transition metal carbide and nitride having high strength, high hardness with large value of cohesive energy. Similarly GaN and AIN are semiconductors which are used in short wavelength electroluminescence devices [11, 12]. The GaN and AIN have been demonstrated as cubic zinc blend structure [13]. In their important experimental observation has pointed out that the bulk glassy rods possess good mechanical properties, the compressive fracture strength and elastic strain to fracture of the amorphous alloy 2, 13 at. % also exhibit ultrahigh fracture strength of 2041 MPa, Young's modulus of 95 GPa [14].

In the present paper the thermo physical properties in terms of compression behaviour of semiconducting materials ($FeSi_2$, SnS, AlN, GaN, MoN,) are investigated by using Tait EOS, Murnaghan EOS, Shanker EOS, and Suzuki EOS under high pressure.

2. Method of analysis

2.1 Tait's Equation of State:

The oldest EOS is called Tait EOS or linear secant (elastic) modulus equation [15, 16] which was formulated as

$$\frac{V}{V_0} = 1 - \frac{aP}{b+P} \tag{1}$$

With $a = \frac{2}{K_0^{'}+1}$ and $b = \frac{2K_0}{K_0^{'}+1}$ and another EOS given by Tait is

$$\frac{V}{V_0} = 1 - a\log(1+bP) \tag{2}$$

With $a = \frac{1}{K_0^{'}+1}$ and $b = \frac{K_0^{'}+1}{K_0}$ (3)

The simplest form of Tait'S EOS for compression and bulk modulus can be expressed as [17]

$$\frac{V}{V_0} = \left[1 - \frac{1}{K_0^{'}+1}\log\left\{1+\left(\frac{K_0^{'}+1}{K_0}\right)P\right\}\right] \tag{4}$$

This is Tait EOS.

2.2 Murnaghan Equation of State:

The well-known and widely used EOS [18] is the Murnaghan EOS which is based on the assumption that isothermal bulk modulus K is linear function of pressure at any temperature that is

$$K(P,T) = K_0 + K_0^{'}P \tag{5}$$

Using the definition of bulk modulus and integrating equation (4) at constant temperature we get the Murnaghan EOS as follows

$$\frac{V}{V_0} = \left(1 + \frac{K_0^{'}}{K_0}P\right)^{\frac{-1}{K_0^{'}}} \tag{6}$$

This is Muenaghan EOS.

2.3 Shanker Equation of State:

The Gruneisen theory of thermal expansion as formulated by Born and Huang has been used by Shanker et al. [19]. These authors included higher order term for the change in volume in the expansion of potential energy and claimed to derive a new expression for V/V_0 which is given by

$$\frac{V}{V_0} - 1 = \frac{1 - \left[1 - 2\left\{\left(K_0^{'} + 1\right)/K_0\right\}P_{Th}\right]^{1/2}}{\left(K_0^{'} + 1\right)} \tag{7}$$

It has been argued by Kushwaha and Shanker that the above EOS may be written as

$$\frac{V}{V_0} - 1 = \frac{1 - \left[1 - 2\left\{\left(K_0^{'} + 1\right)/K_0\right\}(P - P_{Th})\right]^{1/2}}{\left(K_0^{'} + 1\right)} \tag{8}$$

When thermal pressure is zero (P_{Th}=0) then above equation becomes

$$\frac{V}{V_0} = \frac{1 - \left[1 + 2\left\{\left(K_0^{'} + 1\right)/K_0\right\}P\right]^{1/2}}{\left(K_0^{'} + 1\right)} + 1 \tag{9}$$

This is Shanker EOS.

2.4 Suzuki Equation of State:

San-Miguel and Suzuki [20, 21] have followed the Gruneisen theory of thermal expansion based on the Mie Gruneisen equation of state

$$PV + X\left(V\right) = \gamma E_{Th} \tag{10}$$

Where P is pressure, $X\left(V\right) = d\phi / dV,\ \phi$ is potential energy as a function of volume only, γ is the Gruneisen parameter regarded as constant, and E_{Th} is the thermal energy of lattice vibration. After using Taylor's expansion in the second term of equation (9) we get the equation

$$\frac{V}{V_0} = \frac{\left[1 + 2k - \left\{1 - \left(4kE_{Th} / Q\right)\right\}^{1/2}\right]}{2k} \tag{11}$$

In the Mie- Gruneisen EOS

$$P_{Th} = \frac{\gamma E_{Th}}{V_0} \text{ and } Q = \frac{K_0 V_0}{\gamma} \tag{12}$$

Substituting the value P_{Th} and Q in equation (10) we get

$$\frac{V}{V_0} = \frac{1 + 2k - \left\{1 - \left(4kP_{Th}V / K_0V_0\right)\right\}^{1/2}}{2k} \tag{13}$$

Taking $k = \frac{K_0^{'} - 1}{2}$, where $K_0^{'}$ is first pressure derivative of bulk modulus, we get

$$\frac{V}{V_0} = \frac{1 + \left(K_0^{'} - 1\right) - \left[1 - 2\left\{\left(K_0^{'} - 1\right) / K_0\right\} P_{Th}\right]^{1/2}}{\left(K_0^{'} - 1\right)} \tag{14}$$

Where, P_{Th} is thermal pressure. If pressure P is not equal to zero then Equation (12) written as

$$\frac{V}{V_0} = \frac{1 + \left(K_0^{'} - 1\right) - \left[1 - 2\left\{\left(K_0^{'} - 1\right) / K_0\right\}\left(P_{Th} - P\right)\right]^{1/2}}{\left(K_0^{'} - 1\right)} \tag{15}$$

When thermal pressure P_{Th} is equal to zero then above equation becomes

$$\frac{V}{V_0} = \frac{1 - \left[1 + 2\left\{\left(K_0^{'} - 1\right) / K_0\right\} P\right]^{1/2}}{\left(K_0^{'} - 1\right)} + 1 \tag{16}$$

This is Suzuki EOS.

3. Input Parameters

Input parameters with their corresponding references are given in following table:

Table 1: Input parameters with their corresponding references

Solids	**Structure**	**References Temp.(K) Ref.[2, 18-21]**	**K_0(Gpa)**	**K_0'(Gpa)**
$FeSi_2$	Orthorhombic	300	243.45[2]	3.24[2]
SnS	Orthorhombic	300	36.6[18]	5.5[18]
MoN	Simple Hexagonal	300	345[19]	3.5[19]
AlN	Wortzite	300	237[20]	4.7[20]
GaN	Wortzite	300	215.8[21	4.2[21]

4. Results and discussion

In present work an attempt has been made for theoretical calculation of pressure dependence of compression for different semiconductor materials viz. $FeSi_2$, SnS, AlN, GaN, MoN, by using four different isothermal EOS viz. Tait EOS, Murnaghan EOS, Shanker EOS, and Suzuki EOS. The calculated values of compression at different pressure obtained by using equations (3, 5, 8 & 13) are shown in table (2-6) along with experimental values [2, 18-21]. The input values of K_0 and K_0’ taken from literature [2, 18-21] given in table (1).

Table 2**:** Calculated Value of Compressions by using Tait EOS (3), Murnaghan EOS (5), Shanker EOS (8) and Suzuki EOS (13) along with experimental value at different Pressure (GPa) for $FeSi_2$

P	**V/V_0(T)**	**V/V_0(M)**	**V/V_0(Sh)**	**V/V_0(Su)**	**V/V_0(Exp.)[4]**	**%Dev.(T)**	**%Dev.(M)**	**%Dev.(Sh)**	**%Dev.(Su)**
0	1	1	1	1	1	0	0	0	0
5.5	0.9784	0.9784	0.9784	0.9780	0.9756	0.29	0.29	0.29	0.25
13	0.9519	0.9519	0.9516	0.9495	0.9523	0.04	0.04	0.07	0.29
21	0.9265	0.9268	0.9255	0.9208	0.9302	0.40	0.37	0.51	1.01
27	0.9091	0.9096	0.9073	0.9002	0.9090	0.01	0.07	0.19	0.97
35	0.8877	0.8887	0.8845	0.8740	0.8888	0.12	0.01	0.48	1.67
40	0.8753	0.8766	0.8710	0.8582	0.8733	0.23	0.38	0.26	1.73
51	0.8501	0.8522	0.8429	0.8249	0.8510	0.11	0.14	0.95	3.07
60	0.8313	0.8343	0.8213	0.7989	0.8333	0.24	0.12	1.44	4.13

Table 3: Calculated Value of Compressions by using Tait EOS (3), Murnaghan EOS (5), Shanker EOS (8) and Suzuki EOS (13) along with experimental value at different Pressure (GPa) for SnS

P	**V/V_0(T)**	**V/V0(M)**	**V/V0(Sh)**	**V/V_0(Su)**	**V/V_0(Exp.)[4]**	**%Dev.(T)**	**%Dev.(M)**	**%Dev.(Sh)**	**%Dev.(Su)**
0	1	1	1	1	1	0	0	0	0
1.18	0.9707	0.9706	0.9706	0.9698	0.975	0.44	0.45	0.45	0.53
1.86	0.9561	0.9562	0.9556	0.954	0.964	0.82	0.81	0.87	1.04
3.05	0.9334	0.9337	0.9318	0.9283	0.941	0.81	0.78	0.98	1.35
5.25	0.8987	0.8997	0.8935	0.8859	0.920	2.32	2.21	2.88	3.71
5.93	0.8893	0.8906	0.8827	0.8738	0.891	0.19	0.05	0.93	1.93
7.45	0.8703	0.8723	0.8601	0.8483	0.873	0.31	0.08	1.48	2.83
7.62	0.8683	0.8704	0.8577	0.8455	0.8682	0.01	0.25	1.21	2.61
10.5	0.8381	0.8418	0.8193	0.8016	0.8433	0.62	0.18	2.85	4.95
11.86	0.8256	0.8302	0.8026	0.7825	0.8368	1.34	0.79	4.09	6.49
13.56	0.8114	0.8171	0.7828	0.7596	0.8158	0.54	0.16	4.05	6.89
15.27	0.7982	0.8051	0.7639	0.7377	0.8106	1.53	0.68	5.76	8.99
15.93	0.7934	0.8008	0.7569	0.7295	0.7980	0.58	0.35	5.15	8.58

Table 4: Calculated Value of Compressions by using Tait EOS (3), Murnaghan EOS (5), Shanker EOS (8) and Suzuki EOS (13) along with experimental value at different Pressure (GPa) for MoN

P	**V/V_0(T)**	**V/V_0(M)**	**V/V_0(Sh)**	**V/V_0(Su)**	**V/V_0(Exp.)[4]**	**%Dev.(T)**	**%Dev.(M)**	**%Dev.(Sh)**	**%Dev.(Su)**
0	1	1	1	1	1	0	0	0	0
11	0.9702	0.9702	0.9701	0.9693	0.97	0.02	0.02	0.01	0.07
17	0.9555	0.9556	0.9552	0.9534	0.956	0.05	0.04	0.08	0.27
25	0.9373	0.9375	0.9366	0.9331	0.936	0.14	0.16	0.06	0.31
32	0.9225	0.9228	0.9212	0.9161	0.924	0.16	0.13	0.30	0.86
40	0.9067	0.9073	0.9046	0.8973	0.908	0.14	0.08	0.38	1.18
46	0.8956	0.8964	0.8926	0.8836	0.896	0.05	0.05	0.38	1.38
50	0.8884	0.8894	0.8849	0.8747	0.888	0.05	0.16	0.35	1.50
56	0.8781	0.8794	0.8736	0.8616	0.878	0.01	0.16	0.50	1.87
64	0.8651	0.8668	0.8591	0.8447	0.866	0.10	0.09	0.80	2.46
67	0.8604	0.8623	0.8539	0.8384	0.86	0.05	0.27	0.71	2.51
72	0.8528	0.855	0.8452	0.8282	0.856	0.37	0.12	1.26	3.25
74	0.8499	0.8521	0.8418	0.8242	0.85	0.01	0.25	0.97	3.04
80	0.8412	0.8439	0.8318	0.8122	0.844	0.33	0.01	1.45	3.77

Table 5: Calculated Value of Compressions by using Tait EOS (3), Murnaghan EOS (5), Shanker EOS (8) and Suzuki EOS (13) along with experimental value at different Pressure (GPa) for AlN

P	V/V_0(T)	V/V_0(M)	V/V_0(Sh)	V/V0(Su)	V/V_0(Exp.)[4]	%Dev.(T)	%Dev.(M)	%Dev.(Sh)	%Dev.(Su*)
0	1	1	1	1	1	0	0	0	0
2	0.9918	0.9918	0.9918	0.9917	0.99	0.18	0.18	0.18	0.17
6	0.9764	0.9764	0.9763	0.9758	0.975	0.14	0.14	0.13	0.08
7	0.9727	0.9727	0.9726	0.9719	0.97	0.28	0.28	0.27	0.20
10	0.9622	0.9622	0.9619	0.9607	0.96	0.23	0.23	0.20	0.07
15	0.946	0.9461	0.9453	0.9428	0.94	0.64	0.65	0.56	0.30

17	0.9399	0.9401	0.9389	0.9359	0.93	1.07	1.09	0.96	0.64
22.5	0.9242	0.9245	0.9223	0.9176	0.92	0.46	0.49	0.25	0.26

Table 6**:** Calculated Value of Compressions by using Tait EOS (3), Murnaghan EOS (5), Shanker EOS (8) and Suzuki EOS (13) along with experimental value at different Pressure (GPa) for GaN

P	V/V_0(T	V/V_0(M)	V/V_0(Sh)	V/V_0(Su)	V/V_0(Exp.)[4]	%Dev.(T	%Dev.(M)	%Dev.(Sh)	%Dev.(Su*)
0	1	1	1	1	1	0	0	0	0
1	0.9954	0.9954	0.9954	0.9954	0.99	0.55	0.55	0.55	0.55
5	0.9781	0.9781	0.9781	0.9776	0.975	0.32	0.32	0.32	0.27
12	0.9512	0.9513	0.9507	0.9486	0.95	0.13	0.14	0.07	0.15
18	0.9307	0.931	0.9295	0.9255	0.918	1.383	1.42	1.25	0.82
25	0.9093	0.9099	0.9068	0.9001	0.905	0.48	0.54	0.20	0.54
27	0.9036	0.9043	0.9006	0.8932	0.918	1.57	1.49	1.90	2.70
40	0.8702	0.8719	0.8633	0.8504	0.885	1.677	1.48	2.45	3.91
46	0.8566	0.8588	0.8474	0.832	0.875	2.10	1.85	3.15	4.91
52	0.8438	0.8467	0.8322	0.8142	0.85	0.73	0.39	2.09	4.21

- T=Tait EOS, M=Murnaghan EOS, Sh=Shanker EOS, Su = Suzuki EOS

For the sake of comparison the graphical representation of the plots between P and V/V_0 are shown in figure (1-5). The percentage deviations between calculated and experimental values of V/V_0 at different pressure are also shown in table (2-6). On critical analysis of Table (2-6) it is observed that the maximum deviation in calculated values of V/V_0 is 2% for Murnaghan EOS which is least among the other three EOS viz. Tait EOS Shanker EOS and Suzuki EOS. From the Table (2-6) it is also clear that the Suzuki EOS deviates most with experimental values for calculation of compression at different pressure.

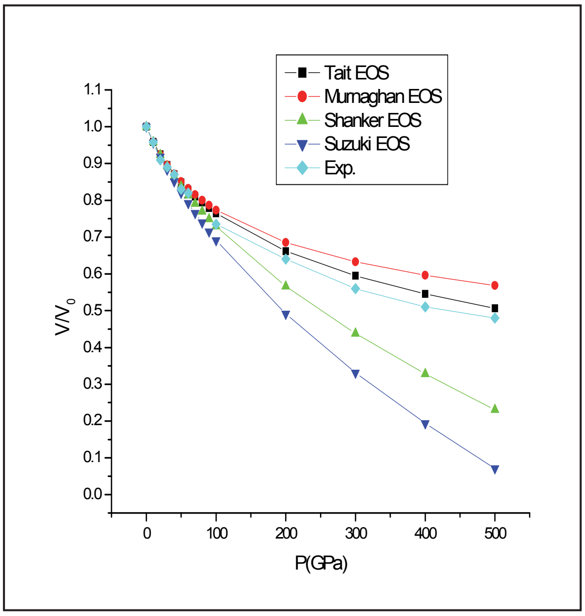

Fig. 1: Compression behavior of $FeSi_2$

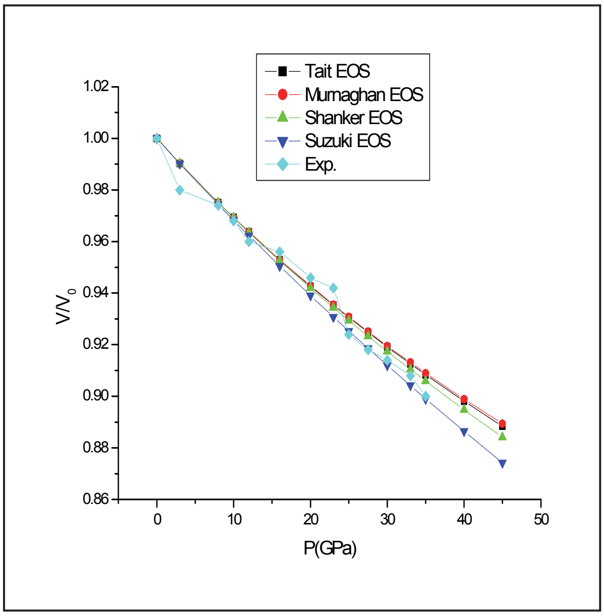

Fig. 2: Compression behavior of SnS

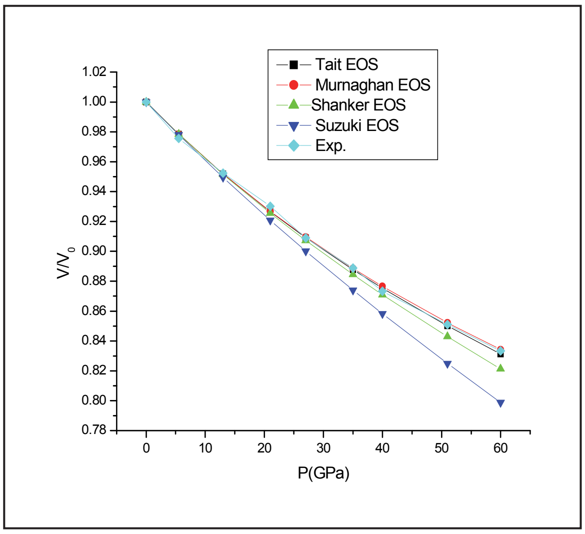

Fig. 3: Compression behavior of MoN

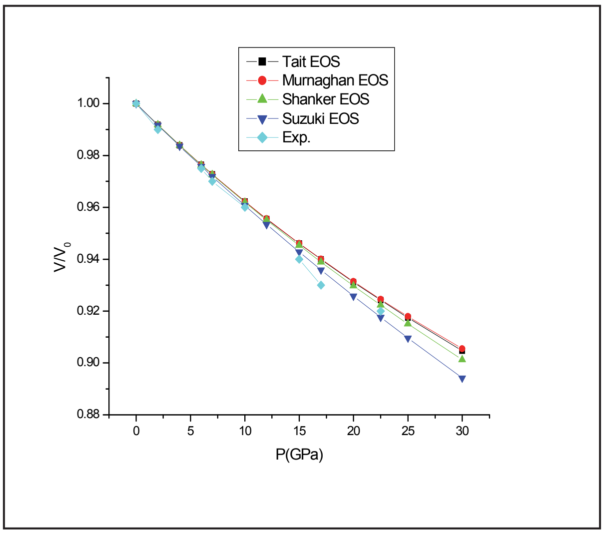

Fig. 4: Compression behavior of AlN

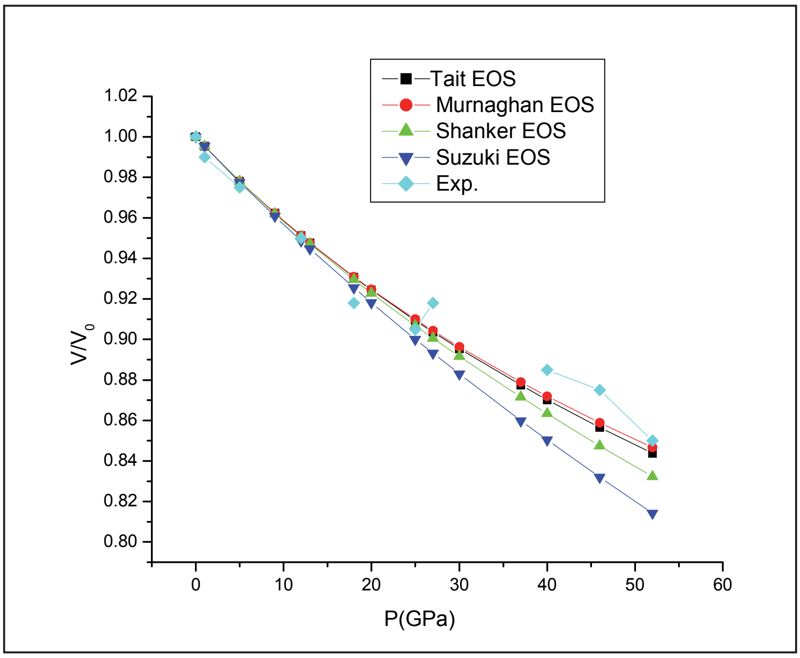

Fig. 5: Compression behavior of GaN

According to the findings of Kamal Devlal [22] Tait equation of state is claimed as the most successful EOS for the explaining the compression behavior of semiconductors. But when we examine the validity of this EOS with others such as Murnaghan EOS, Shanker EOS and Suzuki EOS it is found that the Murnaghan EOS have its consistent validity up to higher pressure range of 80 Gpa. It is also observed that upto low pressure range the Murnaghan EOS leads almost same result as Tait's EOS but at higher pressure range Tait's EOS have much deviation than Murnaghan EOS. The success of Murnaghan EOS for the explanation of compression behavior of semiconductors is due to the fact that its formulation is based on the assumption that isothermal bulk modulus K is linear function of pressure at any temperature. According to Fig. (1-5), it is clear that Murnaghan EOS is the most suitable equation of state for theoretical prediction of compression at different pressure for semiconducting materials.

5. Conclusion

The findings of present work based on theoretical computation of pressure dependence of compression for different semi conducting materials viz. $FeSi_2$, SnS, AlN, GaN, MoN, using different isothermal EOS viz. Tait EOS, Murnaghan EOS, Shanker EOS, and Suzuki EOS. The obtained results are compared with available experimental data which reveals that Murnaghan EOS is most suitable for theoretical prediction of compression for semiconductors at different pressure ranges.

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