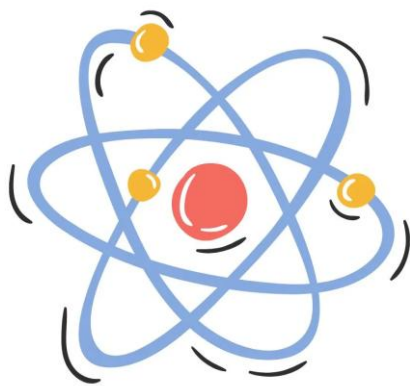




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Abstract – In present the work, we have theoretically calculated some important thermoelastic properties of nanomaterials under high compression, such as pressure, isothermal bulk modulus and percentage deviation of pressure of nanomaterials by using four different Equation of States (EOSs): viz. (I) Birch-Murnaghan EOS, (II) Bardeen EOS (III) Poirier- Tarantola and (IV) Suzuki EOS for 37nm Al_2O_3 , 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials. The result shows that the pressures increase as compression increases, which is in good agreement with experimental value. The bulk modulus also increases as compression increases, and computed value of percentage deviation in pressure at high compression this is demonstrates satisfying result across the entire compression range but the nano- ϵ -Fe nanomaterial percentage deviation shows excellent result with Poirier -Tarantola EOS.

Keywords- High compression, Nanomaterials, Equation of states, Isothermal bulk modules, Grüneisen parameter

Introduction-

Alumina ceramic (Al_2O_3) is known for its fireproof properties. good strength and low thermal expansion coefficient, making it suitable for high temperature structural and substrate applications. Despite these advantages, Al_2O_3 suffer from low ductility and low fracture toughness, prompting the incorporation of metals such as aluminum, cobalt, or alloys into ceramics to enhance their toughness [1-6]. Al_2O_3 is widely utilized in various application such as soft abrasive, catalyst, absorbent, coating, and catalyst carrier. Several synthesis approaches including microwave sintering, high-pressure sintering and plasma-assisted sintering are employed to produce highly dense γ - Al_2O_3 while minimizing excessive grain growth [7-10].

Silicon carbide (SiC) is a high-quality technical grade ceramic belonging to group IV-IV of the periodic table. It exhibits a wide variety of polytypes with unique structural and electronic properties due to the strong covalent bonds formed between silicon (Si) and carbon (C) atoms within its crystal lattice. SiC possesses high strength, a high melting point, high elastic modulus, a wide energy band gap, low thermal expansion, low density, high thermal conductivity and high hardness. Additionally, it demonstrates excellent thermal shock resistance, and chemical inertness. Due to its strength and hardness SiC is used in applications such as vehicles brakes, clutches, and ceramic plates for bullet proof vests [11-12].

In recent years, nano-Ni has garnered more attention to researchers. Researchers have conducted in-depth studies aimed at understanding its properties of such as its electrical behaviors, magnetic mechanics, diffusion coefficient and vibrational modes. Nano-Ni is known for its high conductive and its nanoparticles are available in various forms, including coated and dispersed forms. [13-14].

Iron (Fe) is a highly reactive element to both air and water due to oxygen, and nano-Fe exhibits even higher reactivity compare to bulk Fe. Nano- ϵ -Fe possesses unique physical properties such as ferromagnetic resonance, magnetoelectric coupling and highest coercivity. These

properties find applications in magnetic field-tunable devices and magnetic recording devices. Researchers have conducted extensive investigations into the properties of nano- ϵ -Fe, including surface passivation magnetic, thermal, electrical and mechanical properties, on a large scale [15-29].

In this present work, we calculated the thermoelastic properties viz. Pressure and isothermal bulk modulus at high compression behavior of some nanomaterials viz. 37nm Al_2O_3 , 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials for using isothermal equation of states Suzuki EOS, Birch-Murnaghan EOS, Bardeen EOS, Poirier- Tarantola and Birch-Murnaghan EOS and experimental studies to under the high-pressure behavior of nanomaterials. Further analyze the variation of percentage deviation in pressure under high compression.

Method of analysis- We have investigated the thermoelastic properties of nanomaterials under high compression. Here, we have used four different isothermal EOSs. All the equation of states based on interatomic Potential Model. Which are given below [27, 29-31]:

Suzuki Equation of State-

The Gruneisen theory of thermal expansion based on the Mie-Gruneisen equation of state has followed by San-Miguel and Suzuki. The Mie-Gruneisen equation is written as,

$$PV + X(V) = \gamma E_{Th} \quad (A)$$

In above equation P is pressure, $X(V) = (d\Phi/dV)$, Φ is Potential energy as a volume's function only, γ and E_{Th} is Gruneisen parameter regarded as constant and the thermal energy of lattice vibration. Then after applying Taylor's expansion to the second term in equation (A) with respect to the second order,

$$P = \frac{K_0}{2(K'_0 - 1)} \left[\left\{ \left(\frac{V}{V_0} - 1 \right) (K'_0 - 1) - 1 \right\}^2 - 1 \right] \quad (1)$$

$$K_T = \frac{K_0}{2(K'_0 - 1)} \left[2 \left\{ \left(\frac{V}{V_0} - 1 \right) (K'_0 - 1) - 1 \right\} \left(\frac{V}{V_0} \right) (1 - K'_0) \right] \quad (2)$$

Bardeen Equation of state-

Bardeen EOS The Bardeen equation of state is derived from the potential function $E(r)$ and the Bardeen equation is written as,

$$P = 3K_0 \left[\left(\frac{V}{V_0} \right)^{-\frac{5}{3}} - \left(\frac{V}{V_0} \right)^{-\frac{4}{3}} \right] \left[1 - \frac{3}{2} (K'_0 - 3) \left(\left(\frac{V}{V_0} \right)^{-\frac{1}{3}} - 1 \right) \right] \quad (3)$$

$$K_T = 3K_0 \left[\left\{ \left(\frac{V}{V_0} \right)^{-\frac{5}{3}} - \left(\frac{V}{V_0} \right)^{-\frac{4}{3}} \right\} \left\{ \frac{1}{2} (3 - K'_0) \left(\frac{V}{V_0} \right)^{-\frac{1}{3}} \right\} + \left\{ 1 - \frac{3}{2} (K'_0 - 3) \left(\left(\frac{V}{V_0} \right)^{-\frac{1}{3}} - 1 \right) \right\} \left\{ \frac{1}{3} \left(5 \left(\frac{V}{V_0} \right)^{-\frac{5}{3}} - 4 \left(\frac{V}{V_0} \right)^{-\frac{4}{3}} \right) \right\} \right] \quad (4)$$

Poirier-Tarantola Equation of State-

Poirier and Tarantola derived an equation define strain as $\epsilon = \log(l_0/l)$ and the Poirier-Tarantola EOS is written as,

$$P = K_0 \left(\frac{V_0}{V} \right) \left[\ln \left(\frac{V_0}{V} \right) + \left\{ \left(\frac{K'_0 - 2}{2} \right) \right\} \left\{ \ln \left(\frac{V_0}{V} \right) \right\}^2 \right] \quad (5)$$

$$K_T = K_0 \left(\frac{V_0}{V} \right) \left[1 + (K'_0 - 2) \left\{ \ln \left(\frac{V_0}{V} \right) \right\} \right] + \left[\ln \left(\frac{V_0}{V} \right) + \left\{ \left(\frac{K'_0 - 2}{2} \right) \right\} \left\{ \ln \left(\frac{V_0}{V} \right) \right\}^2 \right] \quad (6)$$

Birch-Murnaghan Equation of state-

Birch-Murnaghan EOS is based on finite strain theory and the Birch-Murnaghan EOS is written as,

$$P = \frac{3}{2} K_0 \left[\left(\frac{V}{V_0} \right)^{-\frac{7}{3}} - \left(\frac{V}{V_0} \right)^{-\frac{5}{3}} \right] \left[1 + \frac{3}{4} (K'_0 - 4) \left(\left(\frac{V}{V_0} \right)^{-\frac{2}{3}} - 1 \right) \right] \quad (7)$$

$$K_T = \frac{K_0}{2} \left[7 \left(\frac{V}{V_0} \right)^{-\frac{7}{3}} - 5 \left(\frac{V}{V_0} \right)^{-\frac{5}{3}} \right] + \frac{3}{8} K_0 (K'_0 - 4) \left(9 \left(\frac{V}{V_0} \right)^{-\frac{9}{3}} - 14 \left(\frac{V}{V_0} \right)^{-\frac{7}{3}} + 5 \left(\frac{V}{V_0} \right)^{-\frac{5}{3}} \right) \quad (8)$$

From above equations (1,3,5 and 7) we can obtain the expression for isothermal bulk modulus (K_T) at pressure (P), by using below mentioned equation

$$K_T = -V \left(\frac{\partial P}{\partial V} \right)_T \quad (B)$$

Result & discussion- In this present work we have described the four different equation of states viz. Suzuki EOS, Bardeen EOS, Poirier-Tarantola EOS and Birch-Murnaghan EOS for calculating the thermoelastic properties of nanomaterials viz. pressure(P), isothermal bulk modulus and percentage deviation in pressure(P) at different compressions for, 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials. The pressure calculated by using equation (1,3,5,7) and isothermal bulk modulus calculated by using equation (2,4,6,8). All the four EOS contain two parameters isothermal bulk modulus and first derivative of isothermal bulk modulus at zero pressure (K_0 and K'_0). It has been usual practice to adjust or to fit the parameters in order to achieve the agreement with the experimental values and its numeric value shown in table 1.

In Table .2, we have seen applicability of Suzuki EOS, Bardeen EOS, Poirier-Tarantola and Birch-Murnaghan EOS for 37nm Al_2O_3 . We have seen that Birch-Murnaghan EOS is slightly deviate from experimental values, so this is best option to calculate pressure at high compression.

In Table .3, we have seen applicability of Suzuki EOS, Bardeen EOS, Poirier-Tarantola and Birch-Murnaghan EOS for 67nm Al_2O_3 . We have seen that Poirier-Tarantola and Birch-Murnaghan EOS are slightly deviate from experimental values, so this is best option to calculate pressure at high compression.

In Table .4, we have seen applicability of Suzuki EOS, Bardeen EOS, Poirier-Tarantola and Birch-Murnaghan EOS for 3C-SiC. We have seen that Poirier-Tarantola and Birch-Murnaghan EOS are slightly deviate from experimental values, so this is best option to calculate pressure at high compression.

In Table .5, we have seen applicability of Suzuki EOS, Bardeen EOS, Poirier-Tarantola and Birch-Murnaghan EOS for Nano-Ni. We have seen that Poirier-Tarantola and Birch-

Murnaghan EOS are slightly deviate from experimental values, so this is best option to calculate pressure at high compression.

In Table .6, we have seen applicability of Suzuki EOS, Bardeen EOS, Poirier-Tarantola and Birch-Murnaghan EOS for Nano- ϵ -Fe. We have seen that Poirier-Tarantola and Birch-Murnaghan EOS are slightly deviate from experimental values, so this is best option to calculate pressure at high compression.

Further finding the value of P we are using the value of K_0 and K'_0 in equation (1,3,5,7). We find the value of K_T Further substituting the values of P and K_T calculated by using equations (2,4,6 and 8). Further we find the value of percentage deviation in P at different compressions. The graphs plotted between the calculated value of P and experimental value of P at different compressions by using Suzuki EOS, Bardeen EOS, Poirier-Tarantola and Birch-Murnaghan EOS are shown in figure (1-5). Further the graphs plotted between calculated value of K_T at different compressions and the graph of K_T are shown in figure (6-10). The calculated value of pressure. Furthermore, the graph of percentage deviation in Pressure (P) at different compression shown in figure (11-15). The equation (1 and 2) represents the Suzuki EOS, the equation (3 and 4) represents the Bardeen EOS, the equation (5 and 6) represents the Poirier-Tarantola EOS and the equation (7-8) represents Birch-Murnaghan EOS respectively.

Table. 1

Input parameters use in this research work.

S.No.	Nanomaterial	K_0	K'_0	Reference
1	37 nm Al_2O_3	151	5.7	[32]
2	67 nm Al_2O_3	248	3.2	[32]
3	3C-SiC	220.6	4	[33]
4	Nano-Ni	185.4	4	[34]
5	Nano- ϵ -Fe	179	3.6	[35]

Table. 2

Calculated value of pressure (P), experimental value of pressure (P) at different compressions for 37 nm Al_2O_3 using (a) Suzuki EOS, (b) Bardeen EOS (c) Poirier- Tarantola and (d) Birch-Murnaghan EOS and percentage deviation in pressure (P)

V/V_0	P(a)	P(b)	P(c)	P(d)	P(exp) [36]	% deviation, P(a)	% deviation, P(b)	% deviation, P(c)	% deviation, P(d)
1	0	0	0	0	0	0	0	0	0
0.98928	1.659499	1.645055	1.677896	1.678214	4.01575	58.67525	59.03492	58.21712	58.20921
0.9197	14.4134	13.72309	15.87178	16.03898	17.85595	19.27954	23.14556	11.11212	10.17569
0.89982	18.68847	17.67206	21.17362	21.52092	22.92747	18.48876	22.92189	7.649564	6.1348

0.882 74	22.585 41	21.263 6	26.258 06	26.848 86	27.882 84	18.998 87	23.739 47	5.8271 67	3.7082 95
0.87 97	25.626 97	24.069 01	30.398 01	31.239 9	31.947 79	19.784 86	24.661 43	4.8509 92	2.2157 57
0.860 06	28.080 04	26.336 32	33.849 23	34.937 2	37.019 3	24.147 57	28.857 86	8.5632 83	5.6243 67
0.850 12	30.603 24	28.675 01	37.505 92	38.891 26	42.419 88	27.856 38	32.401 96	11.584 09	8.3183 2
0.840 18	33.196 55	31.087 51	41.379 39	43.120 92	47.607 54	30.270 39	34.700 44	13.082 27	9.4241 78
0.819 37	38.852 89	36.388 58	50.244 83	52.960 64	51.091 78	23.954 71	28.778 02	1.6576 98	3.6578 54
0.808 65	41.886 62	39.257 94	55.242 67	58.604 65	56.395 58	25.727 12	30.388 27	2.0443 24	3.9170 91

Table. 3

Calculated value of pressure (P), experimental value of pressure (P) at different compressions for 67 nm Al₂O₃ using (a) Suzuki EOS, (b) Bardeen EOS (c) Poirier- Tarantola and (d) Birch-Murnaghan EOS and percentage deviation in pressure (P)

V/V ₀	P(a)	P(b)	P(c)	P(d)	P(exp) [36]	% deviati on, P(a)	% deviati on, P(b)	% deviati on, P(c)	% deviati on, P(d)
1	0	0	0	0	0	0	0	0	0
0.984 21	1.6594 99	4.0102 83	4.0487 9	4.0487 72	5.059	21.250 53	20.729 73	19.968 58	19.968 93
0.954 92	14.413 4	11.974 42	12.311 28	12.310 67	12.949 42	9.3841 58	7.5293 29	4.9279 71	4.9326 23
0.945 08	18.688 47	14.812 62	15.324 86	15.323 65	15.899 5	9.1607 84	6.8359 35	3.6141 95	3.6218 36
0.922 35	22.585 41	21.703 57	22.787 62	22.783 27	23.380 58	10.600 79	7.1726 64	2.5361 09	2.5547 19
0.917 09	25.626 97	23.367 66	24.620 22	24.614 64	25.187 33	10.919 79	7.2245 52	2.2515 81	2.2737 36
0.901 6	28.080 04	28.427 29	30.263 41	30.252 58	30.692 27	11.884 65	7.3796 43	1.3972 87	1.4325 67
0.889 78	30.603 24	32.453 9	34.829 96	34.812 98	35.463 22	13.576 22	8.4857 43	1.7856 75	1.8335 66
0.876 94	33.196 55	36.998 05	40.062 56	40.036 02	40.968 17	15.421 9	9.6907 31	2.2105 21	2.2753 09
0.864 11	38.852 89	41.723 19	45.591 31	45.551 3	46.543 68	16.770 08	10.356 92	2.0461 77	2.1321 4

Table.4

Calculated value of pressure (P), experimental value of pressure (P) at different compressions for 3C-SiC using (a) Suzuki EOS, (b) Bardeen EOS (c) Poirier- Tarantola and (d) Birch-Murnaghan EOS and percentage deviation in pressure (P)

V/V ₀	P(a)	P(b)	P(c)	P(d)	P(exp) [36]	% deviation, P(a)	% deviation, P(b)	% deviation, P(c)	% deviation, P(d)
1	0	0	0	0	0	0	0	0	0
0.99343	1.463625	1.463728	1.473389	1.473422	1.23372	18.63513	18.64344	19.42656	19.42924
0.9898	2.284547	2.284932	2.308408	2.308533	1.87369	21.92768	21.94824	23.20115	23.20782
0.98754	2.800049	2.800752	2.83596	2.836189	3.14907	11.08331	11.06098	9.942933	9.935651
0.98164	4.161759	4.164022	4.241483	4.242229	3.76162	10.63741	10.69756	12.75681	12.77665
0.97528	5.655438	5.660993	5.80344	5.805296	5.83697	3.110041	3.014874	0.574437	0.542642
0.97195	6.448183	6.456324	6.641121	6.643859	6.68723	3.57468	3.452945	0.689504	0.64856
0.95972	9.422646	9.447027	9.838881	9.847287	10.03796	6.12987	5.886979	1.983257	1.899515
0.95357	10.95579	10.99335	11.52142	11.53453	10.80593	1.386868	1.734414	6.621282	6.742623
0.95018	11.8116	11.85814	12.47093	12.48729	12.53386	5.762498	5.391151	0.502097	0.371538
0.94673	12.69035	12.74744	13.45367	13.47388	13.81138	8.116686	7.703383	2.58998	2.443631
0.9434	13.54602	13.6147	14.4182	14.44269	15.03434	9.899483	9.442627	4.098206	3.935315
0.93901	14.68527	14.77156	15.71417	15.74522	16.17715	9.222148	8.688712	2.861932	2.669988
0.93252	16.39286	16.51045	17.6821	17.725	17.50739	6.366067	5.694373	0.99793	1.242934

Table.5

Calculated value of pressure (P), experimental value of pressure (P) at different compressions for nano-Ni using (a) Suzuki EOS, (b) Bardeen EOS (c) Poirier- Tarantola and (d) Birch-Murnaghan EOS and percentage deviation in pressure (P)

V/V ₀	P(a)	P(b)	P(c)	P(d)	P(exp) [36]	% deviation, P(a)	% deviation, P(b)	% deviation, P(c)	% deviation, P(d)
1	0	0	0	0	0	0	0	0	0



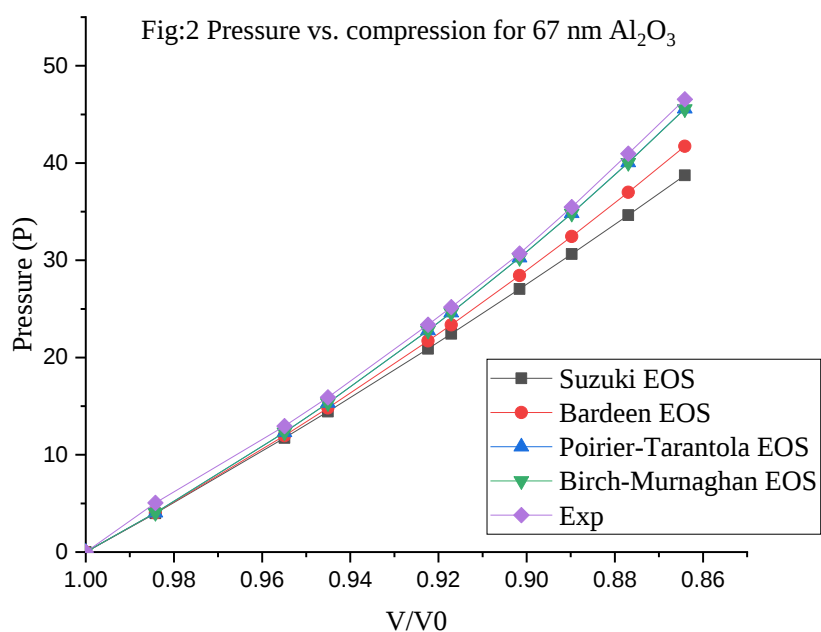
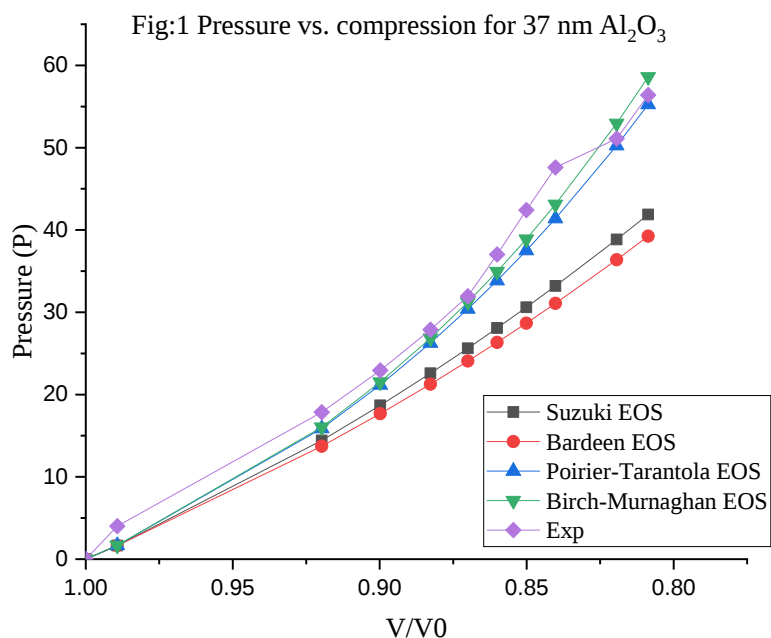
0.995 24	0.8888 05	0.8888 38	0.8930 83	0.8930 93	2.1060 7	57.797 93	57.796 38	57.594 81	57.594 31
0.960 91	7.6722 31	7.6909 38	8.0002 49	8.0066 83	9.7982 6	21.698 03	21.507 11	18.350 31	18.284 64
0.943 74	11.310 84	11.367 52	12.034 19	12.054 38	14.092 66	19.739 48	19.337 33	14.606 71	14.463 42
0.927 28	14.952 94	15.077 24	16.235 08	16.280 92	17.207 29	13.101 16	12.378 76	5.6499 93	5.3835 63
0.900 27	21.255 94	21.584 95	23.909 07	24.037 69	22.162 38	4.0899 72	2.6054 58	7.8813 44	8.4616 63
0.879 87	26.285 42	26.871 88	30.418 58	30.658 46	29.933 21	12.186 42	10.227 19	1.6215 06	2.4228 86
0.868 33	29.233 03	30.013 99	34.400 45	34.728 36	33.142 22	11.795 18	9.4388 12	3.7964 72	4.7858 44
0.855 24	32.666 22	33.717 4	39.199 62	39.654 51	38.632 14	15.442 9	12.721 9	1.4689 43	2.6464 12
0.846 24	35.081 98	36.352 88	42.683 66	43.245 32	43.115 31	18.632 19	15.684 53	1.0011 63	0.3015 39
0.834	38.439 72	40.058 39	47.677 6	48.414 07	51.169 3	24.877 37	21.714 02	6.8238 11	5.3845 42
0.824 15	41.202 34	43.145 49	51.922 2	52.827 56	54.740 1	24.730 98	21.181 2	5.1477 8	3.4938 49

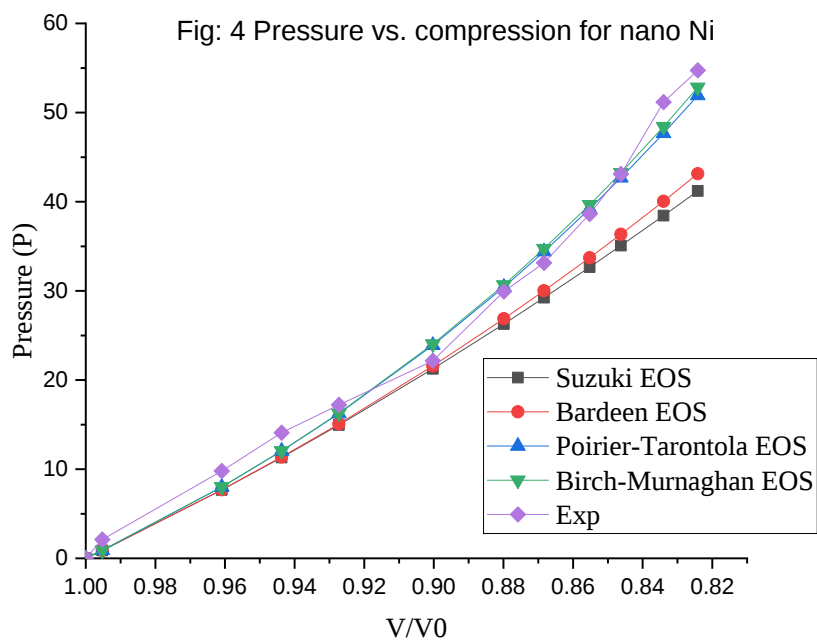
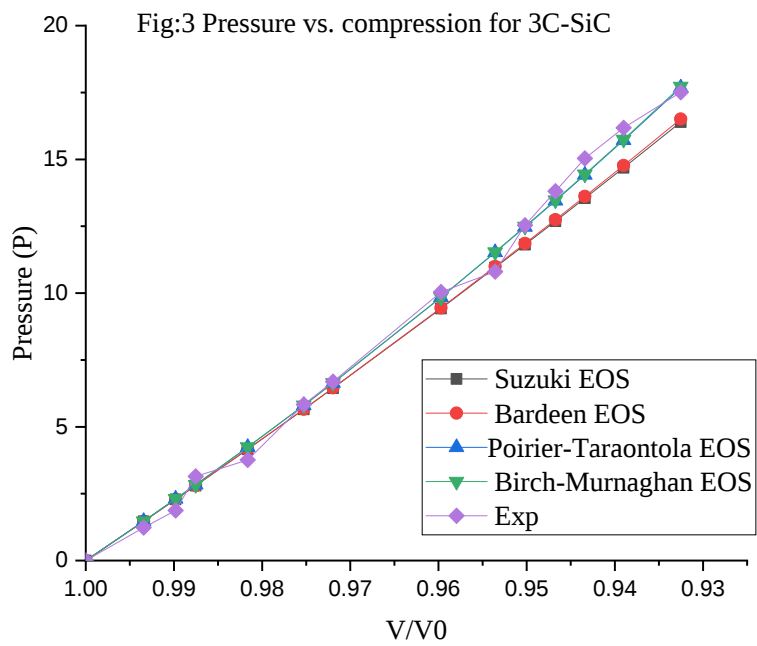
Table.6

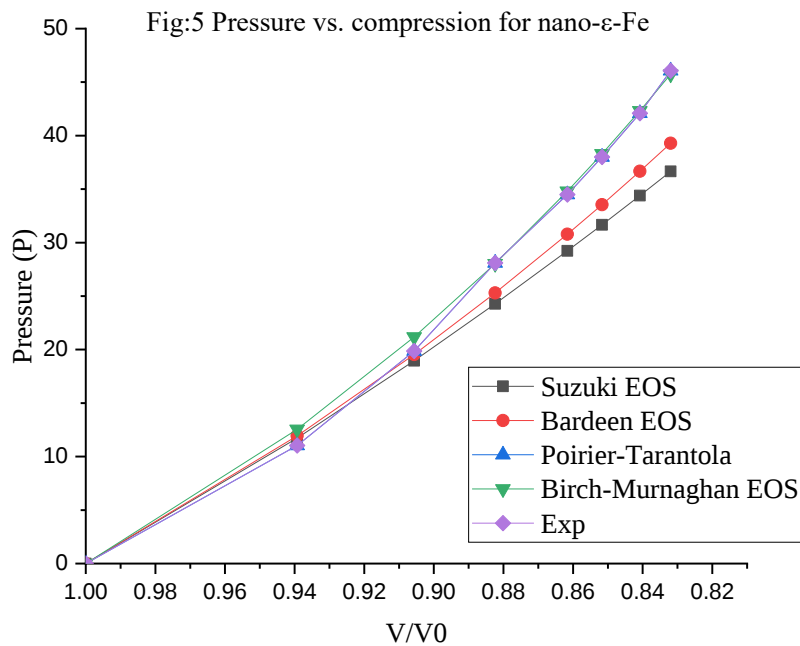
Calculated value of pressure (P), experimental value of pressure (P) at different compressions for nano- ϵ -Fe using (a) Suzuki EOS, (b) Bardeen EOS (c) Poirier- Tarantola and (d) Birch-Murnaghan EOS and percentage deviation in pressure (P)

V/V ₀	P(a)	P(b)	P(c)	P(d)	P(exp) [36]	% deviation, P(a)	% deviation, P(b)	% deviation, P(c)	% deviation, P(d)
1	0	0	0	0	0	0	0	0	0
0.939 25	11.733 04	11.934 35	11.037 74	12.554 86	11.037 74	6.2993 32	8.1231 18	0	13.744 84
0.905 67	18.955 67	19.541 62	19.860 11	21.183 14	19.860 11	4.5540 57	1.6036 42	0	6.6617 24
0.882 37	24.275 6	25.301 26	28.101 79	28.028 52	28.101 79	13.615 48	9.9656 53	0	0.2607 36
0.861 63	29.223 56	30.789 8	34.499 54	34.797 88	34.499 54	15.292 89	10.753	0	0.8647 52
0.851 68	31.668 41	33.551 42	38.004 03	38.293 86	38.004 03	16.670 93	11.716 16	0	0.7626 18
0.840 8	34.394 5	36.671 09	42.089 22	42.315 04	42.089 22	18.281 93	12.872 97	0	0.5365 17
0.831 95	36.652 58	39.288 31	46.062 34	45.747 21	46.062 34	20.428 3	14.706 22	0	0.6841 31

A graph plotted between Pressure with high compression for 37nm Al_2O_3 , 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials are shown in figure (1-5):

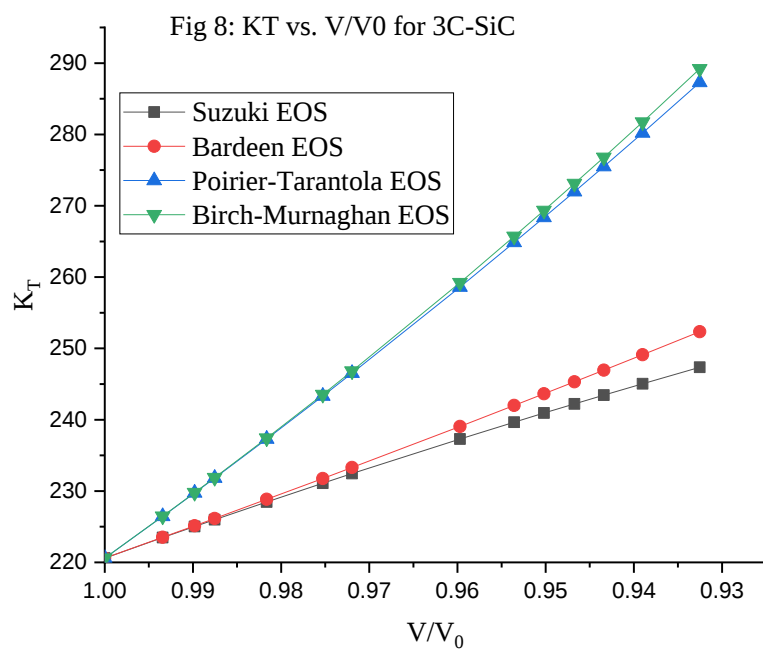
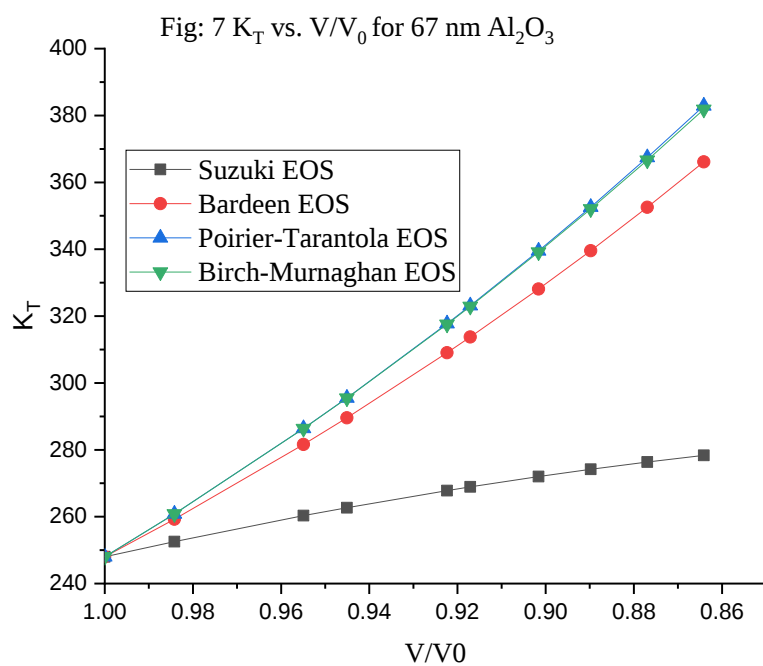


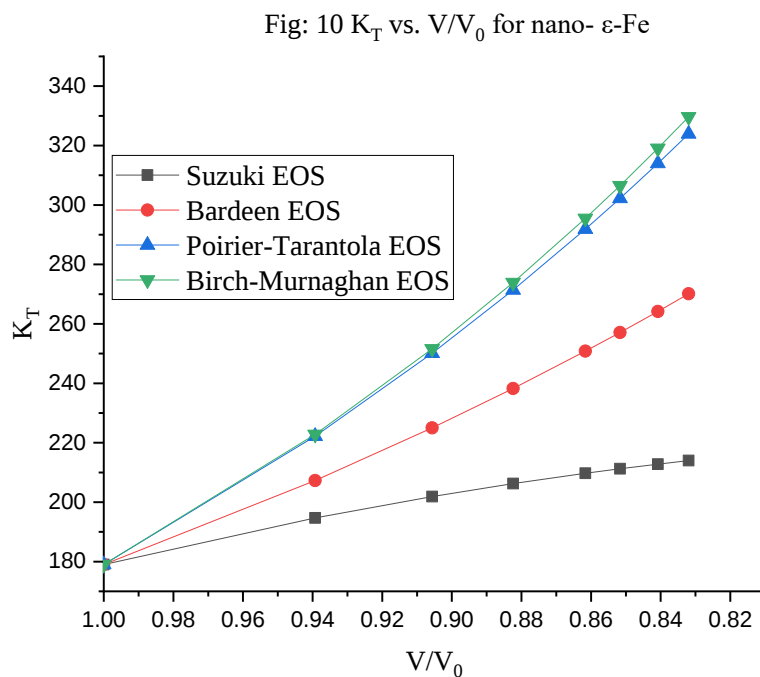
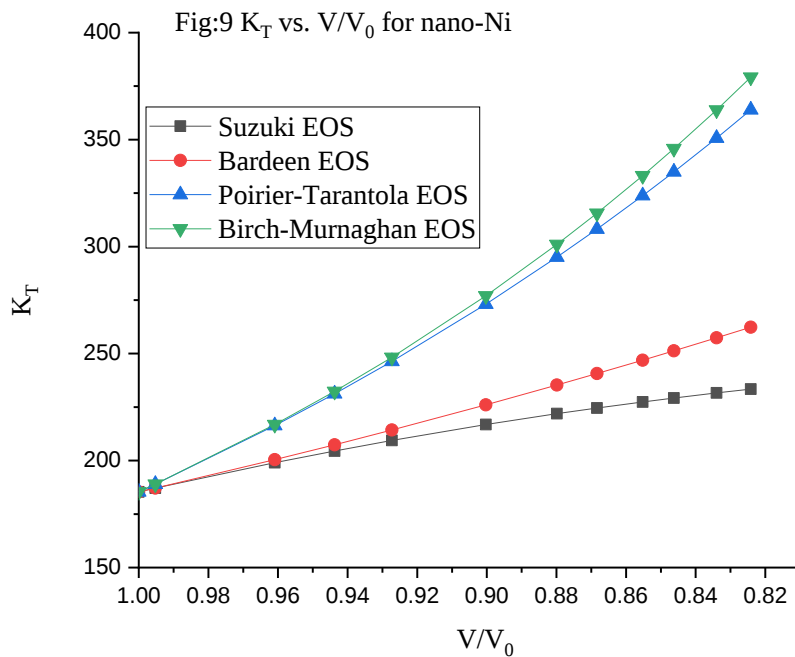




From figure (1-5) it is clear that increasing the pressure leads to an increase in the compression value for all the five nanomaterials viz. 37nm Al_2O_3 , 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials. Furthermore, for 37nm Al_2O_3 the Birch-Murnaghan EOS shows excellent agreement with experimental pressure value. Additionally, for 67nm Al_2O_3 , 3C-SiC and Nano-Ni nanomaterials, both the Birch- Murnaghan EOS and Poirrier – Tarantola EOS demonstrate excellent agreement with the experimental value across the entire range. However, for nano- ϵ -Fe, the Suzuki EOS and Bardeen EOS initially shows good agreement with experimental pressure values up to a volume compression range $(V/V_0) = 0.90$ at 20 GPa, subsequently, the Birch- Murnaghan EOS exhibits excellent agreement with experimental values but Poirier-Tarantola EOS calculated pressure value fully satisfied with experimental values.

A graph plotted between isothermal bulk modulus with high compression for 37nm Al_2O_3 , 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials are shown in figure (6-10):





From figure (6-10) it is clear that an increase in the isothermal bulk modulus (K_T), results in higher compression values across all the five nanomaterials viz. 37nm Al_2O_3 , 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials. For 37nm Al_2O_3 all four EOS exhibit significant differences in the compression range. Similarly, in the case of 67nm Al_2O_3 , the Birch-Murnaghan EOS and Poirier – Tarantola EOS demonstrate good agreement, whereas the Suzuki EOS and Bardeen EOS do not match within the compression range. Conversely, for

3C-SiC, Nano-Ni and nano- ϵ -Fe nanomaterials, the Birch- Murnaghan EOS and Poirrier – Tarantola exhibit excellent agreement throughout the entire range, while the Suzuki EOS and Bardeen EOS do not align within the compression range.

A graph plotted between percentage deviation in pressure (P) with high compression for 37nm Al_2O_3 , 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials are shown in figure (11-15):

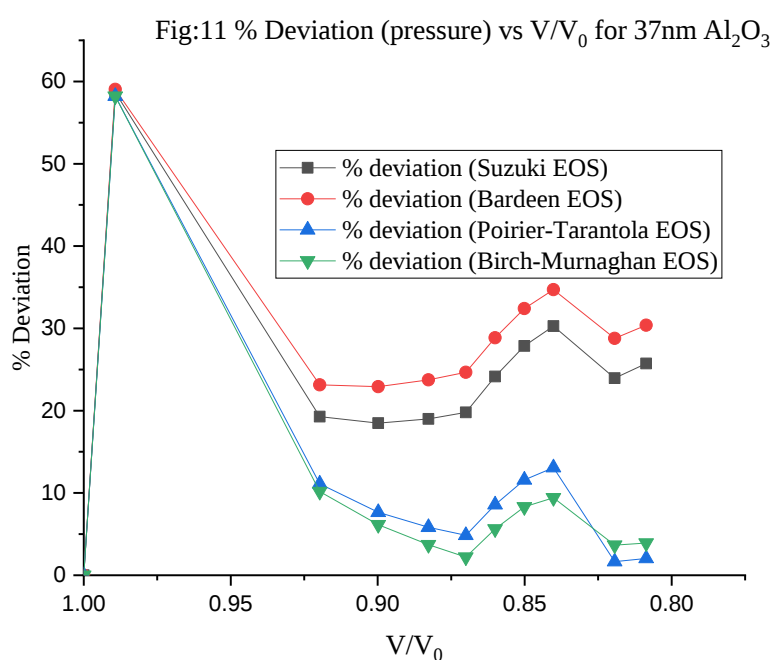


Fig: 12 % Deviation (Pressure) vs V/V_0 for 67 nm Al_2O_3

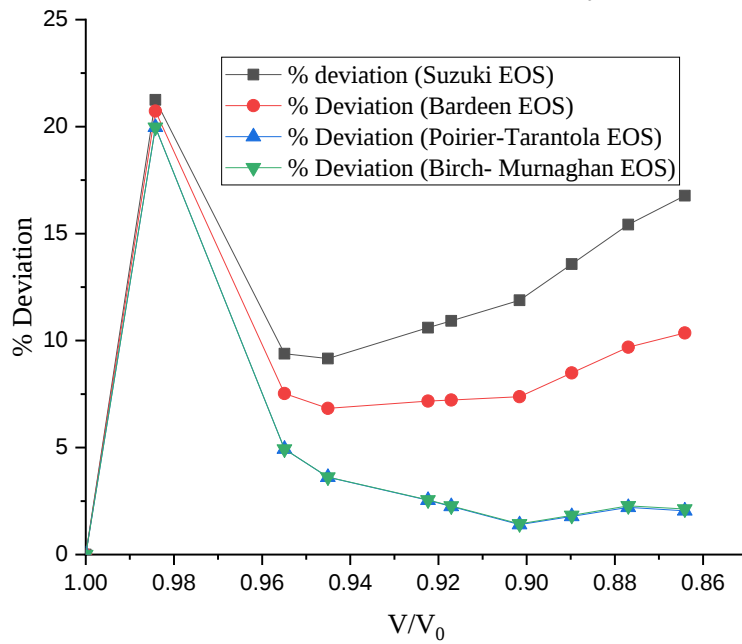
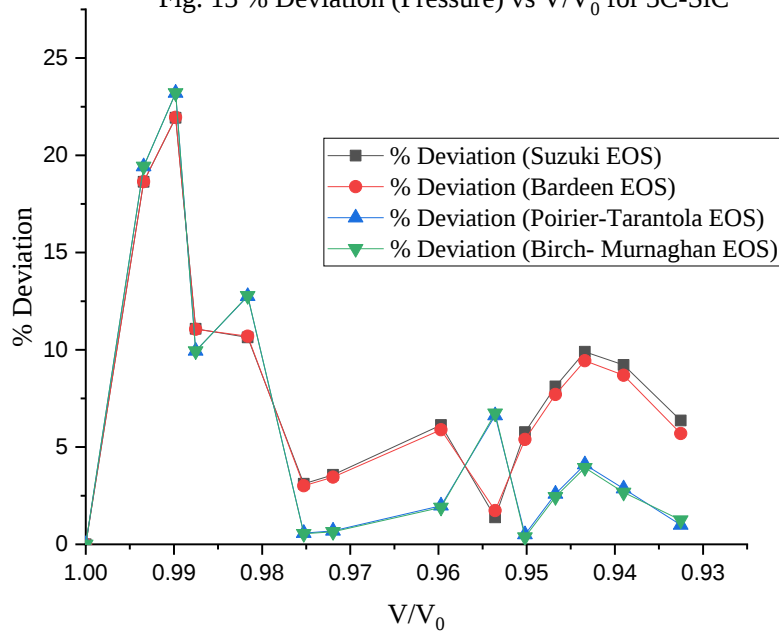
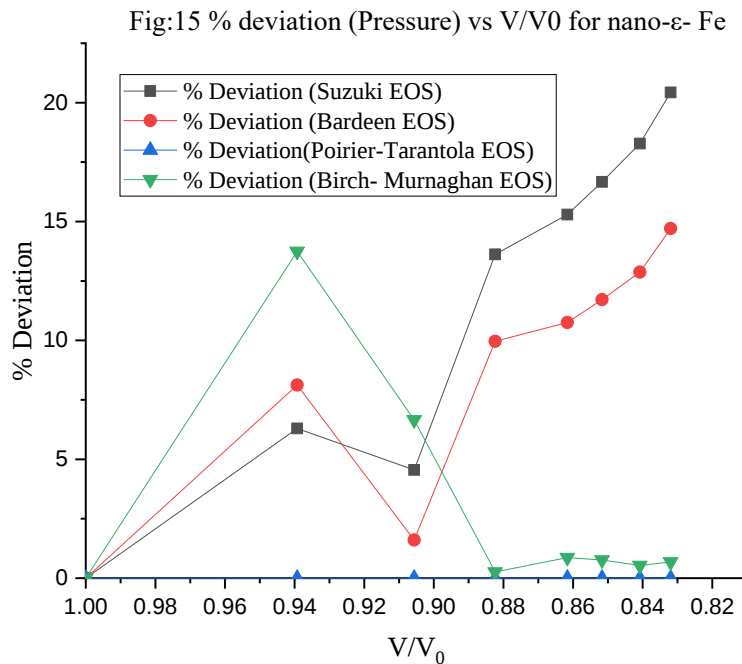
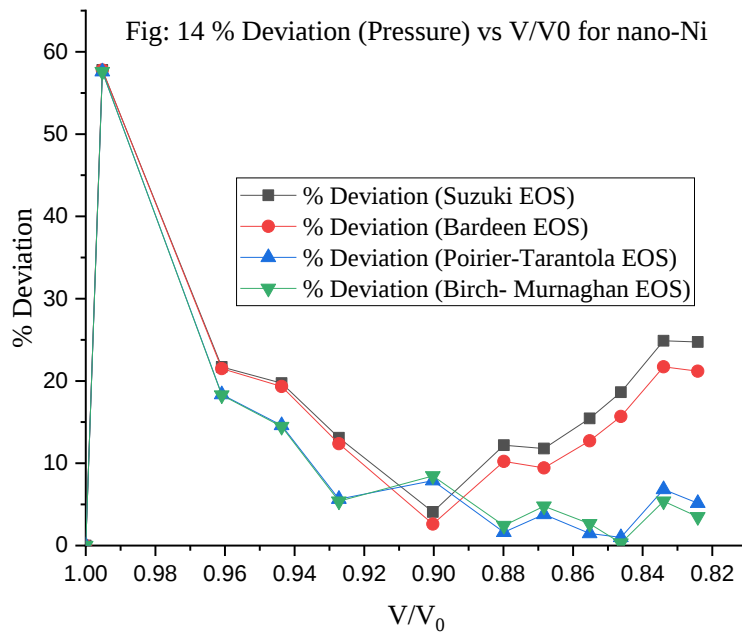


Fig: 13 % Deviation (Pressure) vs V/V_0 for 3C-SiC





From figure (11-15) it is clear that the graph plotted between percentage deviation at various compressions. We have employed four different EOSs viz. Suzuki EOS, Bardeen EOS, Poirier-Tarantola EOS and Birch-Murnaghan EOS. We notice that the Birch-Murnaghan EOS calculated value very close to experimental value, therefore the Birch-Murnaghan EOS is best suitable for 37nm Al_2O_3 comparison to other three EOS. Further, the Poirier-Tarantola EOS and Birch-Murnaghan EOS calculated value very close to experimental value, therefore the

Poirier-Tarantola EOS and Birch-Murnaghan EOS is best suitable for 67nm Al_2O_3 , 3C-SiC and nano-Ni. Furthermore, The Poirier-Tarantola EOS is best suitable for nano- ϵ -Fe because its calculated value fully satisfied with experimental value.

Conclusion- The overall study of thermoelastic properties viz. Pressure and isothermal bulk modulus at high compression for 37nm Al_2O_3 , 67nm Al_2O_3 , 3C-SiC, nano-Ni and nano- ϵ -Fe nanomaterials lead to the conclusion that as pressure increases, compression value increases uniformly across all nanomaterials. It highlights that the Birch-Murnaghan EOS is best suitable for 37nm Al_2O_3 . Additionally, both Poirier-Tarantola EOS and Birch-Murnaghan EOS are best suitable for 67nm Al_2O_3 , 3C-SiC and nano-Ni nanomaterials throughout the range. However, for nano- ϵ -Fe exhibits excellent agreement with experimental value of pressure.

At high compression, increase isothermal bulk modulus for all five nanomaterials. However, there are discrepancies in the behavior of the equations of state (EOS) across different materials. For example, in the case of 37nm Al_2O_3 all four EOS do not coincide throughout the compression range. Conversely, for 67nm Al_2O_3 , the Birch-Murnaghan EOS and Poirier – Tarantola EOS demonstrate good agreement across the entire compression range. Similarly, in the case of

3C-SiC, Nano-Ni and nano- ϵ -Fe nanomaterials, the Birch- Murnaghan EOS and Poirier – Tarantola exhibits excellent agreement throughout the entire range.

Author declaration-

Ethics approval- the author declare that the manuscript is authors own work and has never published elsewhere.

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Reference-

- [1] S. A. Khorrami, M. B. Ahmad, R. Lotfi, K. Shameli, S. Sedaghat, P. Shabanzadeh and M. A. Baghchesara, Digest Journal of Nanomaterials and Biostructures, 7,3, 871-876, (2012)
- [2] C. Toy and W. D. Scott, J. Am. Ceram. Soc. 73, 97, (1990)
- [3] B. D. Flinn, M. Ruhle and A. G. Evans, Acta Metall. 37, 3001, (1989)
- [4] D. C. Halverson, A. J. Pyzik, I. A. Aksay and W. E. Snowden, J. Am. Ceram. Soc. 72, 775, (1988)
- [5] L. S. Sigl and H. F. Fischmeister, Acta Metall. 36, 887, (1988)
- [6] L. Shaw and R. Abbaschian, J. Mater. Sci. 30, 849, (1995)

- [7] J. Freim, J. McKittrick, J. Katz and K. Sickafus, *Nanostruct. Mater.*, 4, 371-385, (1994)
- [8] R. S. Mishra, J.A. Schneider, J. F. Shackelford and A. K. Mukherjee, *Nanostruct. Mater.*, 5, 525-544, (1995)
- [9] M. R. Gallas, B. Hockey, A. Pechenik, and G. J. Piermarini, *J. Am. Ceram. Soc.*, 77, 2107-2112, (1994)
- [10] R. S. Mishra, C. E. Lesher and A. K. Mukherjee, *J. Am. Ceram. Soc.*, 79, 2989-2992, (1996)
- [11] M. E. Levinshtein, S. L. Rumyantsev and M. Shur, Wiley, New York, (2001)
- [12] D. Varshney, S. Shriya, M. Varshney, N. Singh and R. Khenata, *J Theor Appl Phys*, 9, 221-249, (2015)
- [13] J. Rojas-Nunez, S. E. Baltazar, R. I. Gonzalez, E. M. Bringa, S. Allende, M. Kiwi and F. J. Valencia, *nature research*, 10, 21096, (2020)
- [14] E Bonetti, E. G. Campari, L Pasquini and E. Sampaolesi, *J. Appl. Phys.*, 84, 4219-4226, (1998)
- [15] A. K. Pandey, P. Singh, S Srivastava, S. Tripathi and C. K. Dixit, *Thermo Elastic Properties of Nanomaterials under High compression*, 12:2, *J Nanomater Mol Nanotechno*, (2023)
- [16] S Srivastava., A.K Pandey and C K Dixit, *Theoretical prediction for thermoelastic properties of carbon nanotubes (CNTs) at different pressure or compression using equation of states*. *J Math Chem*, 61, 2098-2104 (2023).
- [17] S. Srivastava, A K. Pandey and C K Dixit, *Theoretical prediction of Gruneisen Parameter for Y- Fe₂O₃*, *computational condensed matter*, 35, e00801(2023)
- [18] S Srivastava, C K Dixit and A K Pandey, *Comparative Study of Elastic Properties of Some Inorganic and Organic molecular Crystals by using Isothermal EOS Available at SSRN: <http://ssrn.com/abstract=4427891> or <http://dx.doi.org/10.2139/ssrn.4427891>*, (2023)
- [5] Shivam Srivastava et al., *Equation of states at extreme compression ranges: Pressure and Bulk modulus as an example*, *Materials Open*, doi: 10.1142/S2811086223500073
- [19] A K Pandey, S Srivastava and C K Dixit, *et al.* *Shape and Size Dependent Thermophysical Properties of Nanomaterials*. *Iran J Sci* (2023)
- [20] A.K Pandey, C.K Dixit and S Srivastava, *Theoretical model for the prediction of lattice energy of diatomic metal halides*. *J Math Chem* (2023)
- [21] A Pandey, S Srivastava, & C K Dixit, *A Paradigm Shift in High-Pressure Equation of State Modeling: Unveiling the Pressure–Bulk Modulus Relationship*. *Iran J Sci* (2023)
- [22] AK Pandey, S Srivastava, P Singh, S Tripathi and CK Dixit *Theoretical prediction of Gruneisen parameter for nano Lead Sulfide at different compressions*. (2023) <https://doi.org/10.21203/rs.3.rs-3159558/v1>



- [23] S Srivastava, P Singh, A Pandey and C K Dixit, Solid State communication 377, 115387 (2023)
- [24] A K Pandey, C K Dixit, S Srivastava, P Singh and S Tripathi, Theoretical Prediction of Thermo-Elastic Properties of TiO_2 (Rutile Phase), Natl. Acad. Sci. Lett. (2023)
- [25] S Srivastava, P Singh, A Pandey and C K Dixit, Nano Structure & Nano objects, 36, 101067 (2023)
- [26] S Srivastava, A K Pandey and C K Dixit, Comparative study of elastic properties of some inorganic and organic molecular crystals from EOS. *J Math Chem* (2023).
<https://doi.org/10.1007/s10910-023-01546-9>
- [27] C K Dixit, S Srivastava, P Singh and A K Pandey, nano-structures & nano-objects, 38, 101121, (2024)
- [28] S Srivastava, P Singh, C K Dixit, and A K Pandey, energy storage, 6, e606, (2024)
- [29] S Srivastava, P Singh, A K Pandey and C K Dixit, Analysis of Grunesien Parameter for Carbides and Bromides in Cast Iron, Iranian Journal of science, (2024),
<https://doi.org/10.1007/s40995-024-01602-2>
- [30] D. P. Joshi and A. Senger, Physics Research International, 9, 927324, (2013),
<http://dx.doi.org/10.1155/2013/927324>
- [31] Ibtisam Y. Alkammash, Journal of the Association of Arab Universities for Basic and Applied Sciences, 14, 38–45, (2013)
- [32] B Chen, D Penwell, L R Benedetti, R Jeanloz, and M B Kruger, Phys. Rev. B, 66, 144101-144104, (2002)
- [33] H. H. Liu, J. J. Shu, D. Häusermann and H. Mao, Appl. Phys. Lett., 85(11), 1973-1975, (2004)
- [34] B Chen, D Penwell and MB Kruger, Solid state commun.,115, 191-194, (2000)
- [35] B Chen, D Penwell, MB Kruger, AF Yue and B Fultz, J. of App. Physics, 89, 4794-4796 (2001)
- [36] S. Mishra and A. K. Srivastava, J. Chem. Pharm. Res., 7(6):708-720, (2015)