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EQUATION OF STATE AND BULK MODULUS OF RARE GAS SOLIDS Ne AND Ar

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We have used seven equations of state viz. Lagrangian fourth order EOS, Birch-Murnaghan fourth orders EOS, modified Eulerian EOS, logarithmic fourth order EOS, Vinet-Rydberg EOS, Shanker EOS Hama-Suito EOS. Values of pressure P, isothermal bulk modulus K_T and its pressure derivatives K_T' for Neon and Argon have been calculated down to a compression of 0.50. The results based on different equations are compared with each other and also with the values obtained from the first-principles calculations. It is found that there exists a relationship between the reciprocal of pressure derivative of bulk modulus and the ratio of pressure and bulk modulus. The results have been presented and discussed.

KEYWORDS : Equation of state, Pressure derivative of bulk modulus, Rare gas solids.

INTRODUCTION

The equation of state (EOS) for a material provides useful information for understanding thermodynamic variables such as pressure, temperature and volume. The EOS of condensed matter is very important in the field of geophysics [1-3]. The EOS parameters are determined by using low pressure data such as the equilibrium volume V_0, the isothermal bulk modulus K_0 and pressure derivative K_0' at zero pressure [4]. The fourth-order logarithmic EOS has also been used here to obtain the results for P, K_T and K_T' for two rare gas solids, viz., Ne and Ar for which the first-principle results [5] are available for direct comparison. In the present study we have studied the pressure, bulk modulus and its pressure derivatives for two rare gas solids viz. Ne, Ar at different values of compression V/V_0 down to 0.5. We have used seven EOSs (a) Lagrangian fourth EOS, (b) Birch-Murnaghan fourth-order EOS, (c) Modified Eulerian EOS, (d) Logarithmic fourth-order EOS (e) Vinet-Rydberg EOS, (f) Shanker EOS, (g) Hama-Suito EOS.

It should be mentioned that Ne (fcc) a substance which is most difficult to metallize and Ar (fee) a large gap insulator with a small bulk modulus.

METHOD OF ANALYSIS

We use the following expressions based on different equations of state

2.1. Lagrangian fourth-order EOS

$$P = \frac{9}{16} K_0 \left[A_1 x^{-\frac{1}{3}} - A_2 x^{\frac{1}{3}} + A_3 x - A_4 x^{\frac{5}{3}} \right] \quad \ldots (1)$$

$$K_T = \frac{9}{16} K_0 \left[A_1 \left(\frac{1}{3}\right) x^{-\frac{1}{3}} + A_2 \left(\frac{1}{3}\right) x^{\frac{1}{3}} - A_3 x + A_4 \left(\frac{5}{3}\right) x^{\frac{5}{3}} \right] \quad \ldots (2)$$

$$K'_T = \frac{A_1 \left(\frac{1}{3}\right)^2 x^{-\frac{1}{3}} - A_2 \left(\frac{1}{3}\right)^2 x^{\frac{1}{3}} + A_3 x + A_4 \left(\frac{5}{3}\right) x^{\frac{5}{3}}}{A_1 \left(\frac{1}{3}\right) x^{-\frac{1}{3}} + A_2 \left(\frac{1}{3}\right) x^{\frac{1}{3}} - A_3 x + A_4 \left(\frac{5}{3}\right) x^{\frac{5}{3}}} \quad \ldots (3)$$

where $X = \frac{V}{V_0}$,

$$A_1 = K_0 K''_0 + 3K'_0 + K'^2_0 + \frac{23}{9} \quad \ldots (4)$$

$$A_2 = 3K_0 K''_0 + 7K'_0 + 3K'^2_0 + \frac{7}{3} \quad \ldots (5)$$

$$A_3 = 3K_0 K''_0 + 5K'_0 + 3K'^2_0 - \frac{1}{3} \quad \ldots (6)$$

$$A_4 = K_0 K''_0 + K'_0 + K'^2_0 - \frac{1}{9} \quad \ldots (7)$$

2.2. Birch-Murnughan fourth-order EOS

$$P = \frac{9}{16} K_0 \left[-B_1 x^{-5/3} + B_2 x^{-7/3} - B_3 x^{-3} + B_4 x^{-11/3} \right] \quad \ldots (8)$$

$$K_T = \frac{9}{16} K_0 \left[-B_1 \left(\frac{5}{3}\right) x^{-5/3} + B_2 \left(\frac{7}{3}\right) x^{-7/3} - B_3 (3) x^{-3} + B_4 \left(\frac{11}{3}\right) x^{-11/3} \right] \quad \ldots (9)$$

$$K'_T = \frac{-B_1 \left(\frac{5}{3}\right)^2 x^{-5/3} + B_2 \left(\frac{7}{3}\right)^2 x^{-7/3} - B_3 (3)^2 x^{-3} + B_4 \left(\frac{11}{3}\right)^2 x^{-11/3}}{-B_1 \left(\frac{5}{3}\right) x^{-5/3} + B_2 \left(\frac{7}{3}\right) x^{-7/3} - B_3 (3) x^{-3} + B_4 \left(\frac{11}{3}\right) x^{-11/3}} \quad \ldots (10)$$

where $B_1 = K_0 K''_0 + (K'_0 - 4)(K'_0 - 5) + \frac{59}{9}$ … (11)

$$B_2 = 3K_0 K''_0 + (K'_0 - 4)(3K'_0 - 13) + \frac{129}{9} \quad \ldots (12)$$

$$B_3 = 3K_0K_0'' + \left(K_0' - 4\right)\left(3K_0' - 11\right) + \frac{105}{9} \qquad \ldots (13)$$

$$B_4 = K_0K_0'' + \left(K_0' - 4\right)\left(K_0' - 3\right) + \frac{35}{9} \qquad \ldots (14)$$

2.3. Modified Eulerian EOS

$$P = \frac{9}{2}K_0\left[-D_1x^{-4/3} + D_2x^{-5/3} - D_3x^{-2} + D_4x^{-7/3}\right] \qquad \ldots (15)$$

$$K_T = \frac{9}{2}K_0\left[-D_1\left(\frac{4}{3}\right)x^{-4/3} + D_2\left(\frac{5}{3}\right)x^{-5/3} - D_3\left(2\right)x^{-2} + D_4\left(\frac{7}{3}\right)x^{-7/3}\right] \qquad \ldots (16)$$

$$K_T' = \frac{-D_1\left(\frac{4}{3}\right)x^{-4/3} + D_2\left(\frac{5}{3}\right)^2 x^{-5/3} - D_3\left(2\right)^2 x^{-2} + D_4\left(\frac{7}{3}\right)^2 x^{-7/3}}{D_1\left(\frac{4}{3}\right)x^{-4/3} + D_2\left(\frac{5}{3}\right)x^{-5/3} - D_3\left(2\right)x^{-2} + D_4\left(\frac{7}{3}\right)x^{-7/3}} \qquad \ldots (17)$$

where $$D_1 = K_0K_0'' + \left(K_0' - 3\right)^2 + \frac{26}{9} \qquad \ldots (18)$$

$$D_2 = 3K_0K_0'' + \left(K_0' - 3\right)\left(3K_0' - 8\right) + \frac{66}{9} \qquad \ldots (19)$$

$$D_3 = 3K_0K_0'' + \left(K_0' - 3\right)\left(3K_0' - 7\right) + \frac{60}{9} \qquad \ldots (20)$$

$$D_4 = K_0K_0'' + \left(K_0' - 3\right)\left(K_0' - 2\right) + \frac{20}{9} \qquad \ldots (21)$$

2.4 Logarithmic Fourth-order EOS

Poirier and Tarantola [5] have obtained a third-order logarithmic EOS using the Hencky strain which is represented by 1/3 ln (V/V_0). The loganthmic EOS thus obtained from the free energy expression is

$$P = \frac{1}{V_0}\left(\frac{V}{V_0}\right)\sum_{n=2}^{N}\frac{\left(-1\right)^n nC_n}{3^n}\left(\ln\frac{V_0}{V}\right)^{n-1} \qquad \ldots (22)$$

We obtain in the present study the following expression for the fourth-order logarithmic EOS

$$P = K_0x^{-1}\left[-\left(\ln x\right) + \frac{\left(K_0' - 2\right)}{2}\left(\ln x\right)^2 - \frac{1}{6}Q\left(\ln x\right)^3\right] \qquad \ldots (23)$$

$$K_T = K_0x^{-1}\left[1 - \left(K_0' - 1\right)\left(\ln x\right) + \frac{1}{2}\left(K_0K_0'' + K_0'^2 - 2K_0' + 1\right)\left(\ln x\right)^2 - \frac{1}{6}Q\left(\ln x\right)^3\right] \qquad \ldots (24)$$

$$K_T' = \frac{K_0}{K_T}x^{-1}\left[K_0' - \left(K_0K_0'' + K_0'^2 - K_0'\right)\left(\ln x\right) + \left(K_0K_0'' + K_0'^2 - \frac{5}{2}K_0' + 2\right)\right.$$

$$\left.\left(\ln x\right)^2-\frac{1}{6}Q\left(\ln x\right)^3\right] \quad \ldots (25)$$

where $$Q=\left(K_0K_0''+K_0'^2-3K_0'+3\right) \quad \ldots (26)$$

2.5. Vinet – Rydberg EOS

The expressions for P, K_T, K_T' obtained from this EOS are given below [6, 7]

$$P=3K_0x^{-2/3}\left(1-x^{1/3}\right)\exp\left[\eta\left(1-x^{1/3}\right)\right] \quad \ldots (27)$$

$$K_T=K_0x^{-2/3}\left[1+\left\{\eta x^{1/3}+1\right\}\left(1-x^{1/3}\right)\right]\exp\left[\eta\left(1-x^{1/3}\right)\right] \quad \ldots (28)$$

$$K_T'=\frac{1}{3}\left[\frac{x^{1/3}(1-\eta)+2\eta x^{2/3}}{1+\left(\eta x^{1/3}+1\right)\left(1-x^{1/3}\right)}\right] \quad \ldots (29)$$

where $$\eta=\frac{3}{2}\left(K_0'-1\right)$$

2.6. Shanker EOS

The expression P, K_T, K_T' based on the Shanker EOS are given below [8, 9]

$$P=K_0\frac{x^{-4/3}}{t}\left[\left(1-\frac{1}{t}+\frac{2}{t^2}\right)\left\{\exp\left(ty\right)-1\right\}+y\left(1+y-2/t\right)\exp\left(ty\right)\right] \quad \ldots (30)$$

$$K_T=K_0x^{-1/3}\left(1+y+y^2\right)\exp\left(+y\right)+\frac{4}{3}P \quad \ldots (31)$$

$$K_T'=\frac{4}{3}+\left(1-\frac{4}{3}\frac{P}{K_T}\right)\left[\frac{1}{3}+x\left\{t+\frac{(1+2y)}{\left(1+y+y^2\right)}\right\}\right] \quad \ldots (32)$$

where $t=K_0'-8/3$ and $Y=1-V/V_0$

2.7. Hama-Suito EOS

Hama and Suito [10] have obtained an EOS using first-principles method based on the APW method and QSMs. The expression based on the Hama-Suito EOS are given below

$$P=3K_0x^{-5/3}\left(1-x^{1/3}\right)\exp\left[\frac{3}{2}\left(K_0'-3\right)\left(1-x^{1/3}\right)+\left(z-3/2\right)\left(1-x^{1/3}\right)^2\right] \quad \ldots (33)$$

$$K_T=\frac{P}{3}\left[\left\{5+\frac{x^{1/3}}{\left(1-x^{1/3}\right)}\right\}+x^{1/3}\left\{\frac{3}{2}\left(K_0'-1\right)+2z\left(1-x^{1/3}\right)+3x^{1/3}-6\right\}\right] \quad \ldots (34)$$

$$K_T'=\frac{K_T}{P}-\frac{1}{3}+\frac{P}{9K_T}\left[x^{2/3}\left\{(2z-3)-\frac{1}{\left(1-x^{1/3}\right)^2}\right\}+5\right] \quad \ldots (35)$$

where $$Z = \frac{3}{8}\left(K_0' - 1\right)\left(K_0' + 3\right) + \frac{3}{2}K_0 K_0'' + \frac{1}{3}$$

RESULTS AND DISCUSSIONS

It is found that P and K_T both increase with increase in compression (1 - V/V_0). On the other hand, the pressure derivative of bulk modulus $K' = dK/dP$ decrease with the increase in pressure. These findings are evident from the results given in Table 2 – 7 for Ne and Ar. The results have been obtained from Eqs. 2.1 to 2.7 based on different EOSs using the input data given in Table 1. It is found that the reciprocal of K_T' changes linearly with P/K as given below

$$\frac{1}{K_T'} = a + b\frac{P}{K_T} \qquad \ldots (33)$$

where *a* and *b* are constant for a given material.

The results obtained in the present study compare will with those reported in recent studies [11-14].

Table 1. Values of input data for K_0 (GPa) K_0' and K_0'' (GPa)$^{-1}$ all at $P = 0$, reported by Hama and Suito [10].

Material	K_0	K_0'	K_0''
Ne	6.36	7.61	– 2.86
Ar	6.28	7.07	– 2.53

Table 2. Values of P(GPa) calculated from (a) Lagrangian fourth-order EOS (b) Brich-Murnaghan fourth-order EOS (c) Modified Eulerian EOS (d) Logarithmic fourth order EOS (e) Vinet-Rydberg EOS (f) Shanker EOS (g) Hama-Suito EOS.

For Ne

V/V_0	P (GPa)						
	(a)	(b)	(c)	(d)	(e)	(f)	(g)
1	0	0	0	0	0	0	0
0.95	0.395	0.396	0.396	0.396	0.396	0.396	0.396
0.90	0.984	0.994	0.994	0.992	0.994	1.00	0.994
0.85	1.83	1.89	1.88	1.87	1.89	1.92	1.88
0.80	3.02	3.23	3.22	3.18	3.23	3.31	3.22
0.75	4.65	5.25	5.20	5.08	5.23	5.43	5.21
0.70	6.82	8.31	8.18	7.85	8.24	8.65	8.19
0.65	9.69	13.00	12.67	11.90	12.81	13.59	12.69
0.60	13.46	20.34	19.56	17.86	19.83	21.22	19.60
0.55	18.33	32.09	30.31	26.69	30.80	33.14	30.36
0.50	24.62	51.47	47.48	40.00	48.32	51.94	47.48

For Ar

V/V_0	P (GPa)						
	(a)	(b)	(c)	(d)	(e)	(f)	(g)

1	0	0	0	0	0	0	0
0.95	0.385	0.386	0.386	0.386	0.386	0.386	0.386
0.90	0.946	0.955	0.954	0.953	0.955	0.960	0.954
0.85	1.74	1.79	1.78	1.78	1.79	1.80	1.79
0.80	2.84	3.01	3.00	2.97	3.01	3.07	3.00
0.75	4.33	4.81	4.79	4.69	4.79	4.93	4.78
0.70	6.31	7.47	7.41	7.17	7.43	7.70	7.39
0.65	8.91	11.48	11.33	10.75	11.35	11.85	11.26
0.60	12.3	17.6	17.2	15.9	17.2	18.1	17.0
0.55	16.7	27.1	26.3	23.6	26.3	27.6	25.9
0.50	22.3	42.5	40.6	35.07	40.4	42.3	39.8

Table 3. Values of K_T (GPa) calculated from (a) Lagrangian fourth-order EOS (b) Brich-Murnaghan fourth order EOS (c) Modified Eulerian EOS (d) Logarithmic fourth order EOS (e) Vinet-Rydberg EOS (f) Shanker EOS (g) Hama-Suito EOS.

For Ne

V/V_0	K_T (GPa)						
	(a)	(b)	(c)	(d)	(e)	(f)	(g)
1	6.36	6.36	6.36	6.36	6.36	6.36	6.36
0.95	9.16	9.20	9.19	9.19	9.20	9.25	9.19
0.90	12.7	13.1	13.1	13.0	13.1	13.3	13.1
0.85	17.1	18.5	18.4	18.1	18.5	19.1	18.4
0.80	22.2	26.1	25.8	25.0	26.0	27.2	25.8
0.75	28.2	36.9	36.1	34.2	36.5	38.8	36.2
0.70	35.0	52.5	50.7	46.6	51.5	55.4	50.9
0.65	42.7	75.4	71.6	63.4	72.8	79.1	71.8
0.60	51.3	109.9	102.1	86.3	104.1	113.3	102.3
0.55	60.8	164.4	147.5	118.2	150.5	162.8	147.4
0.50	71.3	249.0	216.9	163.0	221.0	235.3	215.7

For Ar

V/V_0	K_T (GPa)						
	(a)	(b)	(c)	(d)	(e)	(f)	(g)
1	6.28	6.28	6.28	6.28	6.28	6.28	6.28
0.95	8.82	8.85	8.86	8.85	8.86	8.89	8.86
0.90	12.0	12.3	12.3	12.3	12.3	12.5	12.3
0.85	16.0	17.0	17.0	16.8	17.0	17.5	17.0
0.80	20.5	23.5	23.4	22.8	23.5	24.3	23.4
0.75	25.7	32.6	32.2	30.8	32.3	33.8	32.1
0.70	31.7	45.3	44.5	41.4	44.6	47.1	44.2
0.65	38.5	63.6	61.8	55.7	61.9	65.6	61.1

0.60	46.0	90.5	86.9	75.2	86.6	91.7	85.3
0.55	54.0	131.0	123.8	102.0	122.6	128.7	120.5
0.50	63.5	194.1	179.6	139.7	175.9	181.6	172.6

Table 4. Values of K'_T calculated from (a) Lagrangian fourth-order EOS (b) Brich-Murnaghan fourth order EOS (c) Modified Eulerian EOS (d) Logarithmic fourth order EOS (e) Vinet-Rydberg EOS (f) Shanker EOS (g) Hama-Suito EOS.

For Ne

V/V_0	K'_T						
	(a)	(b)	(c)	(d)	(e)	(f)	(g)
1.00	7.61	7.61	7.61	7.61	7.61	7.61	7.61
0.95	6.59	6.84	6.83	6.79	6.85	7.01	6.93
0.90	5.59	6.28	6.23	6.11	6.27	6.51	6.40
0.85	4.72	5.85	5.76	5.54	5.81	6.07	6.01
0.80	4.00	5.50	5.38	5.07	5.43	5.68	5.60
0.75	3.39	5.22	6.06	4.66	5.11	5.32	5.26
0.70	2.89	4.99	4.78	4.30	4.83	4.98	4.90
0.65	2.47	4.79	4.53	4.00	4.57	4.64	4.54
0.60	2.12	4.63	4.32	3.73	4.34	4.33	4.30
0.55	1.81	4.48	4.13	3.49	4.13	4.02	4.09
0.50	1.55	4.35	3.96	3.27	3.93	3.72	3.80

For Ar

V/V_0	K'_T						
	(a)	(b)	(c)	(d)	(e)	(f)	(g)
1.00	7.07	7.07	7.07	7.07	7.07	7.07	7.07
0.95	6.18	6.39	6.38	6.35	6.39	6.52	8.34
0.90	5.29	5.88	5.86	5.76	5.88	6.06	5.81
0.85	4.51	5.48	5.44	5.26	5.46	5.66	5.40
0.80	3.84	5.16	5.09	4.83	5.10	5.29	5.00
0.75	3.28	4.90	4.81	4.47	4.81	4.95	4.90
0.70	2.81	4.68	4.56	4.15	4.54	4.63	4.42
0.65	2.41	4.49	4.35	3.87	4.31	4.32	4.30
0.60	2.06	4.33	4.15	3.62	4.09	4.03	3.95
0.55	1.77	4.18	3.98	3.39	3.89	3.75	3.65
0.50	1.52	4.06	3.83	3.19	3.69	3.47	3.56

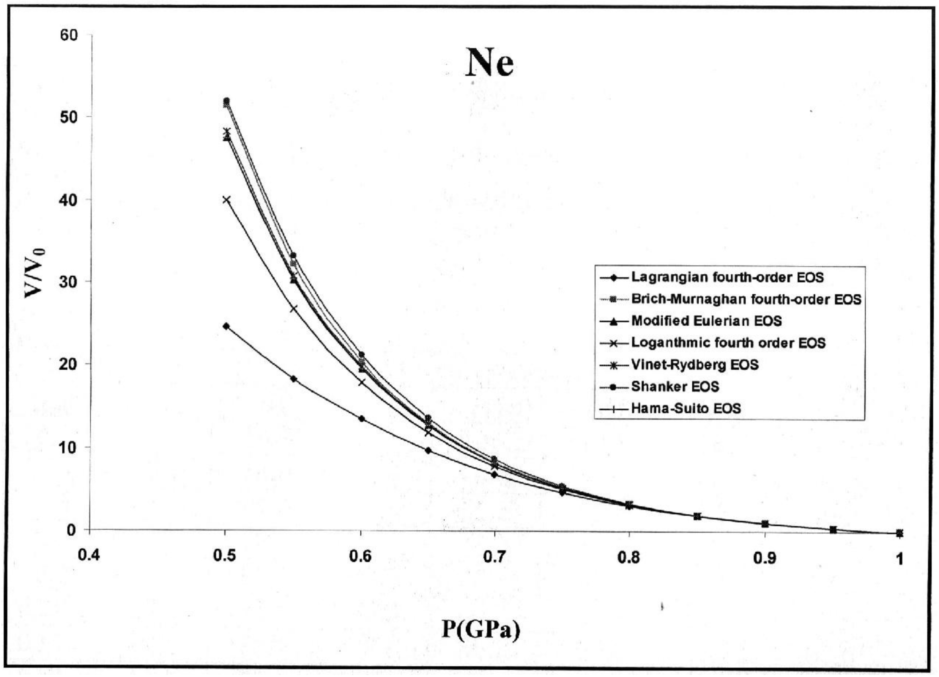

Fig. 1. Pressure versus compression for Ne

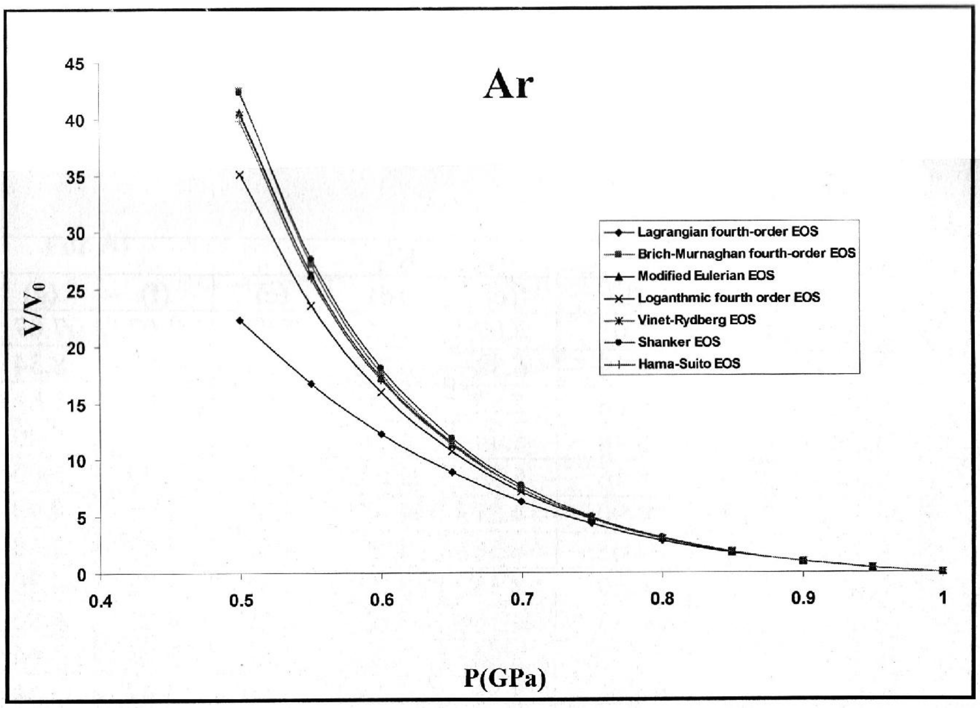

Fig. 2. Pressure versus compression for Ar

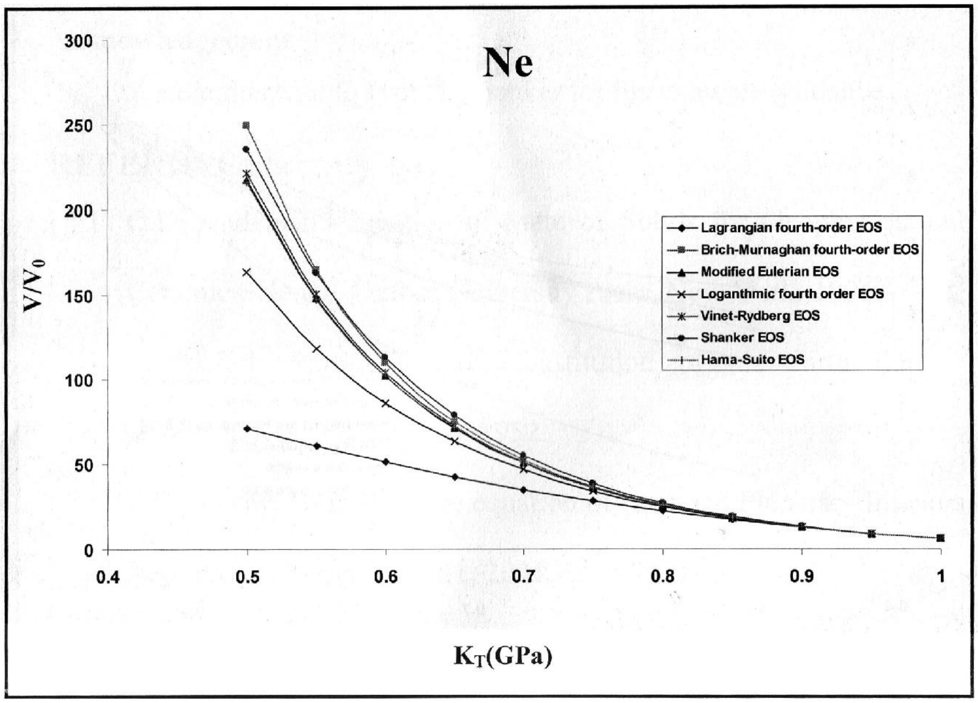

Fig. 3. Isothermal bulk modulus versus compression for Ne

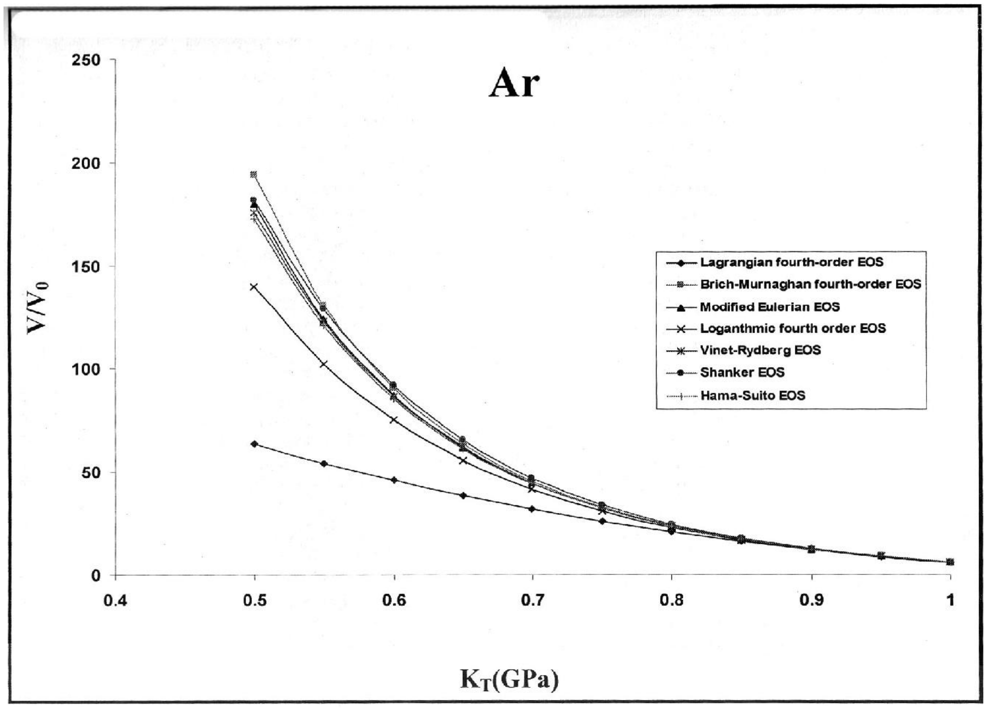

Fig. 4. Isothermal bulk modulus versus compression for Ar

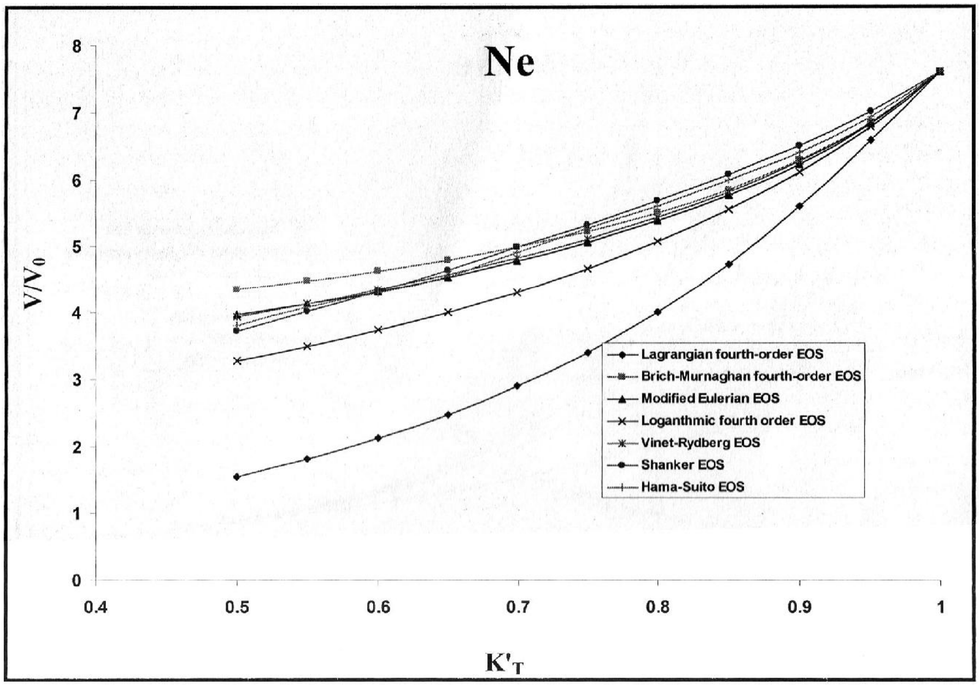

Fig. 5. Pressure derivatives versus compression for Ne

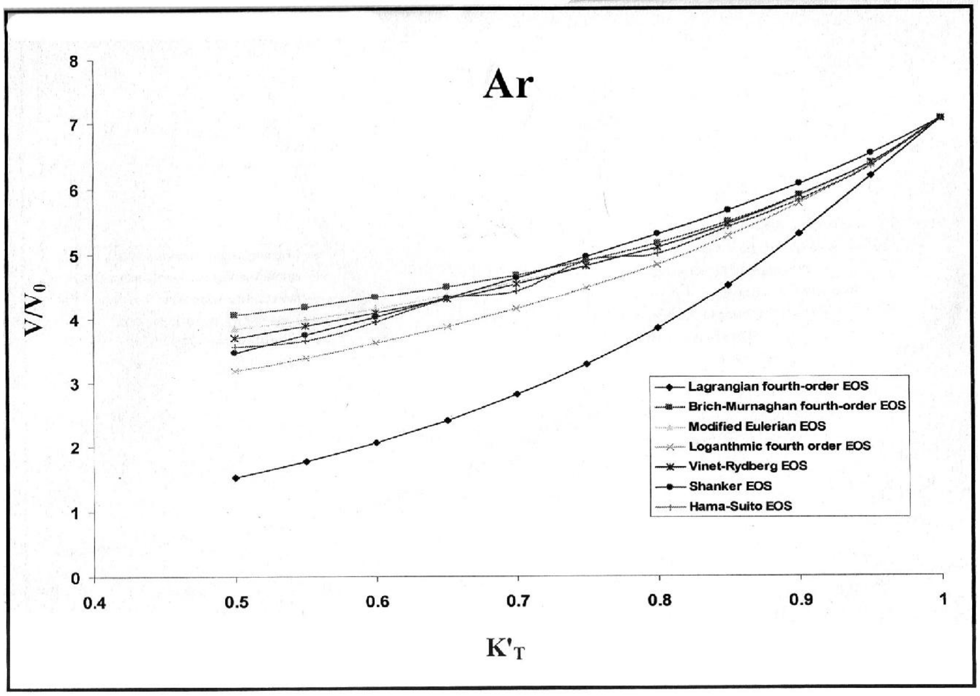

Fig. 6. Pressure derivatives versus compression for Ar

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