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THE STUDY OF HIGH PRESSURE PROPERTIES PHENOMENA OF METALS BY EQUATIONS OF STATE APPROACH

R.S. SINGH AND PREETI SEN

Department of Physics, Faculty of Science, J.N.V. University, Jodhpur (Rajasthan).

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We have studied some high pressure properties of metals using various equation of state. The calculation have been performed using modified Rydberg EOS (equation of state), Hama Suito EOS, Stacey Reciprocal K-prime EOS, Kushwah logarithmic EOS, Kushwah Exponential EOS to find the pressure, bulk modulus and its pressure derivative for seven metals at different values of compression V/V_0. The results for various parameters show systematic variations with the increase in pressure and compare well with the Stacey EOS.

KEYWORDS: Equation of state, metals, pressure, bulk modulus.

INTRODUCTION

The equation of state (EOS) of a system describes the relationship among thermodynamic variables such as pressure, temperature and volume [1, 3]. The study of equation of state for solid have been extremely useful in the field of Geophysics and condensed matter Physics [4,7].

The EOS's have been derived by many authors based on different physical assumption. Among these EOS's its very difficult to choose appropriate EOS. Among these EOS's we have chosen the equation of state depend on free volume theory [8]. Equations involving K-primed are more advantageous for determining pressure derivative of bulk modulus than the pressure volume relationship [11-15].

In the present study we determine the pressure, bulk modulus and its pressure derivative for seven metals viz, Ag, Cu, Au, Al, Ta, W and Mo at different values of compression V/V_0 (from 0.8 to 1.0).

We have used five EOS's (a) Modified Rydberg EOS, (b) Hama Suito EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS, (e) Kushwah Exponential EOS.

The results for different metals obtained from these Eos's have been found to present good agreement with experimental data [6,9,10].

EQUATION OF STATE

The equation of state used in the present study are

(a) Modified Rydberg EOS[2,17]

$$P = 3K_0 x^{-K'_\infty}\left(1 - x^{1/3}\right)\exp\left[t\left(1 - x^{1/3}\right)\right]$$

$$K = 3K_0 x^{-K'_\infty}\exp\left\{t\left(1 - x^{1/3}\right)\right\}\left\{K'_\infty\left(1 - x^{1/3}\right)\right\} + \frac{t}{3}\left\{x^{1/3}\left(1 - x^{1/3}\right)\right\} + \frac{x^{1/3}}{3}$$

$$K' = K'_\infty + t\frac{x^{1/3}}{3} + \frac{x^{1/3}}{3\left(1 - x^{1/3}\right)} - \frac{P}{9K}tx^{1/3} + \frac{1}{1 - x^{1/3}} + \frac{x^{1/3}}{\left(1 - x^{1/3}\right)^2}$$

where $x = \frac{V}{V_0}$

$$\mathrm{t} = \frac{3}{2}K'_0 - 3K'_\infty + \frac{1}{2}$$

Here K_0, K'_0 and K''_0 are respectively zero pressure values of K, K'_0, K''_0 and K'_∞ is the value of K' at $P \to \infty$.

(b) Hama Suito EOS [3,17]

$$P = 3K_0 x^{-K'_\infty}\left(1 - x^{1/3}\right)\exp\left[A\left(1 - x^{1/3}\right) + B\left(1 - x^{1/3}\right)^2\right]$$

$$K = \frac{P}{3}\left\{3K'_\infty + \frac{x^{1/3}}{1 - x^{1/3}}\right\} + x^{1/3}\left\{A + 2B\left(1 - x^{1/3}\right)\right\}$$

$$K' = \frac{K}{P} - \frac{1}{3} + \frac{P}{9K}\left\{3K'_\infty + \left(x^{1/3}\right)^2 2B - \frac{1}{\left(1 - x^{1/3}\right)^2}\right\}$$

where $x = \frac{V}{V_0}$

$$A = (3/2)\left(\mathrm{K}'_0 - 2K'_\infty + 1/3\right)$$

$$B = (3/8)\left(4K_0K''_0 + {K'_0}^2 + 2\mathrm{K}'_0 - 4K'_\infty + 5/9\right)$$

(c) Stacey Reciprocal *k*-primed EOS [4,17]

$$\log\frac{V}{V_0} = \frac{K'_0}{{K'_\infty}^2}\log\left(1 - K'_\infty\frac{P}{K}\right) + \left(\frac{\mathrm{K}'_0}{K'_\infty} - 1\right)\frac{P}{K}$$

$$K = K_0\left(1 - K'_\infty\frac{P}{K}\right)^{-\frac{K'_0}{K'_\infty}}$$

$$\frac{1}{K'} = \frac{1}{K'_0} + \left(1 - \frac{K'_\infty}{K'_0}\right)\frac{P}{K}$$

(d) Kushwah Logarithmic EOS [5,17]

$$Px^{K'_\infty} = B_1 \log(2-x) + B_2\left[\log(2-x)\right]^2 + B_3\left[\log(2-x)\right]^3$$

$$K = K'_\infty P + \frac{x^{1-K'_\infty}}{2-x}\left[B_1 + 2B_2 \log(2-x) + 3B_3\left\{\log(2-x)^2\right\}\right]$$

$$K' = 2K'_\infty - \frac{K'^{\,2}_\infty P}{K} + \frac{2}{2-x}\left[\frac{K'_\infty P}{K} + \frac{x^{2-K'_\infty}}{K(2-x)}\left\{B_2 + 3B_3 \log(2-x)\right\} - 1\right]$$

where $\quad x = 1 - \dfrac{V}{V_0}$

$$B_1 = K_0$$

$$B_2 = \left(\frac{K_0}{2}\right)\left(K'_0 - 2K'_\infty + 2\right)$$

and $\quad B_3 = \left(\dfrac{K_0}{6}\right)\left(K_0 K''_0 + K'^{2}_0 + 3K'^{\,2}_\infty - 3K'_\infty K'_\infty - 12K'_\infty + 6K'_0 + 6\right)$

(e) Kushwah Exponential EOS [6]

$$(1-x)^{K'_\infty} = B_1\left(1-e^{-x}\right) + B_2\left(1-e^{-x}\right)^2 + B_3\left(1-e^{-x}\right)^3$$

$$K = K'_\infty P + \frac{e^{-x}}{(1-x)^{K'_\infty - 1}}\left[B_1 + 2B_2 \log\left(1-e^{-x}\right) + 3B_3\left\{\left(1-e^{-x}\right)^2\right\}\right]$$

$$K' = 2K'_\infty + x - 2 - K'_\infty\left(x + K'_\infty - 2\right)\frac{P}{K} + \frac{e^{-2x}}{K(1-x)^{K'_\infty - 2}}\left[2B_2 + 6B_3\left(1-e^{-x}\right)\right]$$

where $\quad x = 1 - \dfrac{V}{V_0}$

$$B_1 = K_0$$

$$B_2 = \left(\frac{K_0}{2}\right)\left(K'_0 - 2K'_\infty + 2\right)$$

and $\quad B_3 = \left(\dfrac{K_0}{6}\right)\left(K_0 K''_0 + K'^{2}_0 + 3K'^{\,2}_\infty - 3K'_0 K'_\infty - 12K'_\infty + 6K'_0 + 6\right)$

We make use of these equations to calculate values of pressure.

Results and discussion

Values of input parameters used in the present calculation are given in table 1. We determine pressure P for seven metals.

Table 1.

Values of input data for different metals at room temperature and zero pressure [18,19, 20]

Metals	Ag	Cu	Au	Al	Ta	W	Mo
K_0	99.65	133.4	166.7	72.67	191.4	306.0	268.0
K'_0	6.11	5.37	6.00	4.62	3.81	4.17	3.58
K'_∞	3.67	3.22	3.60	2.77	2.29	2.50	2.14
$K_0\ K''_0$	–14.93	–11.53	–14.40	–8.54	–5.81	–6.96	–5.12

Table 2.

Values of pressure for the different metals calculated from (a) Modified Rydberg EOS, (b) Hama Suito EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS, (e) Kushwah Exponential EOS

Metals	V/V_0	P				
		(a)	(b)	(c)	(d)	(e)
Ag	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	2.14	2.14	2.14	2.14	2.14
	0.96	4.61	4.60	4.60	4.60	4.60
	0.94	7.45	7.42	7.43	7.42	7.42
	0.92	10.73	10.65	10.67	10.66	10.66
	0.90	14.50	14.34	14.37	14.37	14.36
	0.88	18.85	18.55	18.62	18.61	18.61
	0.86	23.87	23.35	23.50	23.47	23.47
	0.84	29.67	28.81	29.07	29.04	29.03
	0.82	36.38	35.03	35.48	35.43	35.41
	0.80	44.15	42.11	42.82	42.76	42.74
Cu	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	2.82	2.84	2.85	2.85	2.84
	0.96	5.97	6.07	6.08	6.07	6.06
	0.94	9.48	9.72	9.73	9.72	9.72
	0.92	13.42	13..85	13.86	13.85	13.85
	0.90	17.82	18.52	18.53	18.53	18.53
	0.88	22.75	23.78	23.82	23.83	23.82
	0.86	28.28	29.72	29.83	29.82	29.81

	0.84	34.50	36.42	36.62	36.61	36.59
	0.82	41.49	43.97	44.29	44.31	44.28
	0.80	49.37	52.48	53.04	53.05	53.00
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	3.58	3.58	3.57	3.58	3.57
	0.96	7.69	7.68	7.68	7.68	7.68
	0.94	12.42	12.38	12.38	12.38	12.38
	0.92	17.86	17.75	17.77	17.76	17.75
Au	0.90	24.11	23.87	23.91	23.91	23.90
	0.88	31.31	30.85	30.95	30.94	30.92
	0.86	39.60	38.79	38.99	38.97	38.95
	0.84	49.15	47.82	48.21	48.16	48.14
	0.82	60.18	58.09	58.73	58.68	58.65
	0.80	72.92	70.92	70.82	70.74	70.69
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	1.54	1.54	1.54	1.53	1.53
	0.96	3.26	3.26	3.26	3.25	3.25
	0.94	5.19	5.18	5.18	5.17	5.17
	0.92	7.35	7.32	7.32	7.32	7.32
Al	0.90	9.77	9.71	9.73	9.72	9.71
	0.88	12.49	12.37	12.40	12.40	12.39
	0.86	15.55	15.34	15.38	15.39	15.38
	0.84	18.98	18.66	18.74	18.74	18.73
	0.82	22.86	22.35	22.48	22.50	22.48
	0.80	27.22	26.48	26.70	26.71	26.68
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	4.02	4.02	4.03	4.01	4.01
	0.96	8.45	8.44	8.44	8.44	8.44
	0.94	13.33	13.31	13.32	13.30	13.30
	0.92	18.71	18.67	18.66	18.66	18.66
Ta	0.90	24.66	24.56	24.57	24.56	24.56
	0.88	31.24	31.05	31.07	31.07	31.06
	0.86	38.52	38.19	38.22	38.24	38.22
	0.84	46.59	46.06	46.12	46.15	46.12
	0.82	55.54	54.74	54.88	54.90	54.84
	0.80	65.49	64.30	64.53	64.57	64.48
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	6.45	6.45	6.45	6.44	6.44
	0.96	13.60	13.59	13.59	13.59	13.59

	0.94	21.54	21.51	21.49	21.51	21.50
	0.92	30.36	30.28	30.27	30.28	30.28
W	0.90	40.17	39.99	40.01	40.00	40.00
	0.88	51.09	50.74	50.77	50.79	50.77
	0.86	63.26	62.65	62.72	62.76	62.72
	0.84	76.83	75.85	76.00	76.05	75.99
	0.82	91.98	90.45	90.74	90.82	90.73
	0.80	108.94	106.65	107.17	107.28	107.13
	1.00	0.00	0.00	0.00	0.00	0.00
	0.98	5.61	5.61	5.61	5.61	5.61
	0.96	11.71	11.76	11.77	11.75	11.75
	0.94	18.33	18.48	18.56	18.48	18.47
	0.92	25.95	25.83	25.92	25.85	25.82
Mo	0.90	34.11	33.86	34.07	33.91	33.86
	0.88	43.09	42.64	43.02	42.75	42.66
	0.86	52.99	52.23	52.88	52.44	52.28
	0.84	63.91	62.69	63.71	63.07	62.83
	0.82	75.97	74.13	75.68	74.16	74.40
	0.80	89.32	86.61	88.90	87.61	87.10

Table 3.

Values of bulk modulus and pressure derivative of bulk modulus for the different metals calculated from (a) Modified Rydberg EOS, (b) Hama Suito EOS, (c) Stacey reciprocal *K*-primed EOS, (d) Kushwah logarithmic EOS, (e) Kushwah Exponential EOS

Metals	V/V_0	K					K'				
		(a)	(b)	(c)	(d)	(e)	(a)	(b)	(c)	(d)	(e)
	1.00	99.65	0.00	99.65	99.65	99.65	0.00	0.00	6.11	6.11	6.11
	0.98	112.55	112.41	12.39	112.42	112.42	5.94	5.82	5.83	5.83	5.83
	0.96	127.55	126.41	126.48	126.49	126.48	5.79	5.57	5.61	5.60	5.60
	0.94	143.28	141.79	142.08	142.03	142.01	5.65	5.34	5.41	5.40	5.40
	0.92	161.58	138.67	159.34	159.25	159.21	5.52	5.13	5.25	5.23	5.23
Ag	0.90	182.19	177.22	178.49	178.38	178.32	5.41	4.93	5.10	5.09	5.08
	0.80	205.48	197.60	199.89	199.71	199.61	5.30	4.76	4.97	4.96	4.95
	0.86	231.03	220.01	223.90	223.54	223.40	5.20	4.59	4.86	4.84	4.84
	0.84	2.61.70	244.65	250.71	250.26	250.06	5.11	4.44	4.76	4.74	4.74
	0.82	295.65	271.78	280.89	280.28	280.01	5.02	4.29	4.66	4.65	4.65
	0.80	334.33	301.67	314.87	314.13	313.78	4.94	4.16	4.58	4.57	4.57
	1.00	133.40	0.00	133.41	133.41	133.40	0.00	0.00	5.37	5.37	5.37

	0.98	145.90	148.38	148.39	148.37	148.35	4.39	4.16	5.15	5.15	5.15
	0.96	159.60	164.69	164.73	164.70	164.67	4.32	4.96	4.97	4.97	4.97
	0.94	174.66	182.45	182.62	182.53	182.53	4.25	4.77	4.81	4.81	4.81
	0.92	191.22	201.80	202.23	202.13	202.13	4.18	4.60	4.68	4.68	4.67
Cu	0.90	209.48	222.90	223.77	223.69	223.69	4.12	4.45	4.55	4.56	4.55
	0.88	229.64	245.92	247.59	247.48	247.48	4.06	4.30	4.45	4.45	4.44
	0.86	251.94	271.05	274.03	273.79	273.49	4.00	4.17	4.35	4.36	4.34
	0.84	276.66	298.51	303.29	302.98	302.98	3.95	4.04	4.26	4.27	4.26
	0.82	304.11	328.54	333.68	335.03	335.44	3.90	3.92	4.18	4.20	4.18
	0.80	334.67	361.40	371.94	372.44	371.64	3.85	3.81	4.11	4.13	4.11
	1.00	166.70	0.00	166.7	166.7	166.7	0.00	0.00	6.00	6.00	6.00
	0.98	187.87	187.68	187.65	187.66	187.66	5.84	5.73	5.73	5.73	5.73
	0.96	211.57	210.68	210.74	210.72	210.71	5.69	5.49	5.51	5.51	5.51
	0.94	238.14	235.91	236.18	236.17	236.14	5.55	5.26	5.32	5.32	5.31
	0.92	268.00	263.59	264.49	264.32	264.27	5.43	5.06	5.15	5.16	5.15
Au	0.90	301.59	293.96	295.75	295.57	295.57	5.32	4.87	5.01	5.02	5.00
	0.88	339.45	327.31	330.65	330.35	330.17	5.21	4.70	4.88	4.89	4.88
	0.86	382.22	363.94	369.59	369.16	368.90	5.11	4.53	4.77	4.78	4.76
	0.84	430.63	404.19	413.25	412.60	412.22	5.02	4.38	4.68	4.68	4.67
	0.82	485.55	448.43	462.04	461.36	460.84	4.94	4.24	4.59	4.59	4.58
	0.80	548.00	497.19	517.15	516.24	515.56	4.86	4.11	4.51	4.51	4.50
	1.00	72.67	0.00	72.67	72.67	72.67	0.00	0.00	4.62	4.62	4.62
	0.98	79.70	79.63	79.65	79.64	79.64	4.52	4.45	4.46	4.46	4.46
	0.96	87.41	87.15	87.19	87.21	87.19	4.43	4.30	4.32	4.32	4.31
	0.94	95.87	95.26	95.38	95.37	95.36	4.35	4.16	4.20	4.19	4.19
	0.92	105.18	104.02	104.28	104.26	104.24	4.27	4.03	4.09	4.08	4.08
Al	0.90	115.43	113.50	113.98	113.96	113.91	4.19	3.91	4.00	3.99	3.98
	0.88	126.74	123.75	124.58	124.51	124.46	4.12	3.79	3.91	3.90	3.89
	0.86	139.24	134.85	136.19	136.03	136.01	4.06	3.68	3.83	3.82	3.82
	0.84	153.08	146.89	148.95	148.72	148.67	4.00	3.58	3.77	3.74	3.74
	0.82	168.44	159.94	162.99	162.61	162.59	3.94	3.49	3.70	3.67	3.68
	0.80	185.51	174.13	178.49	178.00	177.44	3.88	3.40	3.65	3.61	3.62
	1.00	191.4	0.00	191.39	191.39	191.40	0.00	0.00	3.81	3.81	3.81
	0.98	206.59	206.50	206.47	206.50	206.47	3.75	3.70	3.70	3.70	3.69
	0.96	223.04	222.65	222.61	222.60	222.61	3.68	3.60	3.60	3.60	3.59
	0.94	240.88	239.91	239.93	239.95	239.90	3.63	3.50	3.51	3.51	3.58
	0.92	260.25	258.40	258.55	258.51	258.47	3.57	3.41	3.43	3.43	3.42
Ta	0.90	281.32	278.21	278.62	278.55	278.45	3.52	3.32	3.35	3.36	3.35
	0.88	304.27	299.45	300.30	300.15	299.98	3.46	3.23	3.29	3.30	3.28

	0.86	329.31	322.26	323.75	323.45	323.25	3.42	3.15	3.22	3.24	3.21
	0.84	356.68	346.78	349.19	348.74	348.43	3.37	3.08	3.17	3.18	3.15
	0.82	386.64	373.16	376.85	376.26	375.75	3.32	3.01	3.11	3.13	3.10
	0.80	419.50	401.59	406.97	406.10	405.45	3.28	2.94	3.06	3.04	3.05
	1.00	306.00	0.00	306.00	306.00	306.10	0.00	0.00	4.17	4.17	4.17
	0.98	332.61	332.44	332.46	332.45	332.44	4.09	4.04	4.03	4.03	4.03
	0.96	361.58	360.81	360.86	360.89	360.86	4.01	3.91	3.92	3.92	3.92
	0.94	393.17	391.29	391.45	391.55	391.45	3.94	3.79	3.82	3.82	3.81
	0.92	427.66	424.05	424.57	424.19	424.53	3.88	3.68	3.72	3.73	3.72
W	0.90	465.39	459.29	460.44	460.58	460.28	3.82	3.58	3.64	3.65	3.63
	0.88	506.71	497.23	499.19	499.56	499.03	3.76	3.48	3.56	3.57	3.55
	0.86	552.05	538.13	541.35	541.97	541.14	3.70	3.39	3.49	3.51	3.48
	0.84	601.89	582.26	587.33	588.24	586.99	3.65	3.31	3.42	3.45	3.42
	0.82	656.77	629.92	637.42	638.83	637.03	3.60	3.22	3.36	3.39	3.36
	0.80	717.33	681.45	692.34	694.28	691.78	3.55	3.15	3.31	3.34	3.31
	1.00	268.00	0.00	268.0	268.0	268.00	0.00	0.00	3.57	3.58	3.58
	0.98	287.93	287.81	287.8	287.81	287.81	3.52	3.48	3.48	3.48	3.48
	0.96	309.44	308.92	308.8	308.95	308.94	3.47	3.39	3.39	3.39	3.39
	0.94	332.67	331.44	331.5	331.57	331.51	3.41	3.30	3.31	3.31	3.30
	0.92	357.81	355.49	355.8	355.81	355.67	3.36	3.22	3.24	3.24	3.23
Mo	0.90	385.06	381.19	381.7	381.85	381.56	3.31	3.14	3.17	3.17	3.16
	0.88	414.62	408.68	409.7	409.84	409.36	3.27	3.06	3.11	3.12	3.09
	0.86	446.74	438.11	439.7	440.03	439.26	3.22	2.99	3.05	3.06	3.03
	0.84	481.71	469.67	472.2	472.65	471.49	3.18	2.92	3.00	3.01	2.98
	0.82	519.84	503.54	507.3	507.96	506.30	3.14	2.86	2.95	2.96	2.93
	0.80	561.50	539.93	545.40	546.27	543.97	3.10	2.80	2.90	2.92	2.88

Conclusion

To conclude, results obtained for seven metals (Ag, Cu, Au, Al, Ta, W and Mo) using the input data (table 1) are reported in tables (2 & 3) for pressure, bulk modulus and its pressure derivative at different values of V/V_0 (from 0.8–1.0).

It is found that these equations for pressure, bulk modulus and its pressure derivative yield results which are most identical with the corresponding values obtained from the Stacey reciprocal *K*-primed EOS for all metals.

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