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# Temperature-dependent equation of state of condensed matter

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**Abstract.** In the present paper, a temperature-dependent equation of state (EOS) of condensed matter is discussed, which is capable of predicting the high-pressure and high-temperature behaviour of solids and liquids. The EOS can be used to obtain the volume compression, the isothermal bulk modulus and its first pressure derivative, the thermal expansion coefficient and the Anderson–Grüneisen parameter, together with other thermodynamic properties as functions of pressure at different temperatures. The present EOS has been applied for Au, Mo and W and liquid Hg. Good agreement between theory and experiment is observed.

## 1. Introduction

The equation of state (EOS) of condensed matter ( $P$ – $V$ – $T$  relation) is very important in many fields of basic and applied sciences including physics and geophysics. However, many different forms of isothermal EOS ( $P$ – $V$  relation) are available in the literature [1–4] but have been found to have limited uses as far as the practical applications are concerned. Hence, there is a need for a temperature-dependent EOS which will have a wide scope in practical applications in physics and geophysics.

On the one hand, we find the temperature-dependent EOS given by Vinet *et al* [5] and another given by Parsafar and Mason [6]. On the other hand, Kumari and Dass [4] have suggested an EOS which is applicable to a large class of solids [7] and liquids [8]. Therefore, it will be of much interest to see the validity and the usefulness of this EOS after adding thermal effects to make it a temperature-dependent EOS. Hence, the aim of the present paper is to suggest a temperature-dependent EOS which is successful in the high-pressure and high-temperature regions.

## 2. Theory

The EOS given by Kumari and Dass [4] can alternatively be written at a reference temperature  $T_R$  as

$$V(P, T_R)/V(0, T_R) = [(1 + \beta) \exp(ZP) - \beta]^{-1/\eta} \quad (1)$$

The other relations obtained during the development of the EOS are

$$B_T(P, T_R) = B_T(0, T_R) + \frac{B'_T(0, T_R)}{Z} [1 - \exp(-ZP)] \quad (2)$$

and

$$B'_T(P, T_R) = B'_T(0, T_R) \exp(-ZP). \quad (3)$$

In equations (1)–(3),  $B'_T(0, T_R)$  is the first pressure derivative of the isothermal bulk modulus  $B_T(P, T_R)$  at  $P = 0$ ,  $Z$  is a pressure-independent parameter,  $\beta = B'_T(0, T_R)/[B_T(0, T_R)Z]$  and  $\eta = B'_T(0, T_R) + B_T(0, T_R)Z$ .

To include the thermal effects into the EOS, we use the simplest form

$$P(T) = P(T_R) + \alpha(0, T_R)B_T(0, T_R)(T - T_R) \quad (4)$$

where  $\alpha(0, T_R)$  is the thermal expansion coefficient. Equation (4) has been used extensively (see, e.g., [5, 6, 9]).

Putting equation (4) into equations (1)–(3), we get

$$V(P, T)/V(0, T_R) = [(1 + \beta) \exp \sigma - \beta]^{-1/\eta} \quad (5)$$

$$B_T(P, T) = B_T(0, T_R) + \frac{B'_T(0, T_R)}{Z} [1 - \exp(-\sigma)] \quad (6)$$

and

$$B'_T(P, T) = B'_T(0, T_R) \exp(-\sigma) \quad (7)$$

where  $\sigma$  is taken as

$$\sigma = Z[P - \alpha(0, T_R)B_T(0, T_R)(T - T_R)]$$

under the condition that  $Z$  is also a temperature-independent parameter.

Thus, equation (5) represents a temperature-dependent EOS of condensed matter and will be tested in solids and liquids to determine its validity at high pressures and high temperatures.

The following important results can be obtained from equations (5)–(7).

(i) Equation (5) can also be written as

$$P = \frac{1}{Z} \ln \left( \frac{(V(P, T)/V(0, T_R))^{-\eta} + \beta}{1 + \beta} \right) + \alpha(0, T_R)B_T(0, T_R)(T - T_R). \quad (8)$$

Thus, the main advantage of the present EOS given by equation (5) is that it is an inverted EOS, i.e. we can write the volume as a function of pressure and temperature ( $V = f(P, T)$ ) given by equation (5) or the pressure as a function of volume and temperature ( $P = f(V, T)$ ) given by equation (8). Hence, the present EOS definitely has the advantage over all those EOSs which are non-invertible but can be expressed in many forms.

(ii) Together with  $V(P, T)$ , we can also study simultaneously  $B_T(P, T)$  and  $B'_T(P, T)$  as functions of both the pressure and the temperature with the help of equations (6) and (7), respectively.

(iii) Differentiation of equation (8) with respect to temperature at constant volume taking  $Z$  as the temperature-independent parameter gives

$$\left( \frac{\partial P}{\partial T} \right)_V = \alpha(P, T)B_T(P, T) = \alpha(0, T_R)B_T(0, T_R). \quad (9)$$

Equation (9) represents the same results which have already been obtained by Kumari and Dass [10] from quite a different approach. Many interesting results can be obtained with the help of equation (9) and a few are listed here.

(a) Both the thermal expansion coefficient  $\alpha(P, T)$ , and the Anderson–Grüneisen parameter  $\delta_T(P, T)$  can be studied as functions of pressure at different temperatures [11].

(b) An isobaric EOS can be obtained [10].

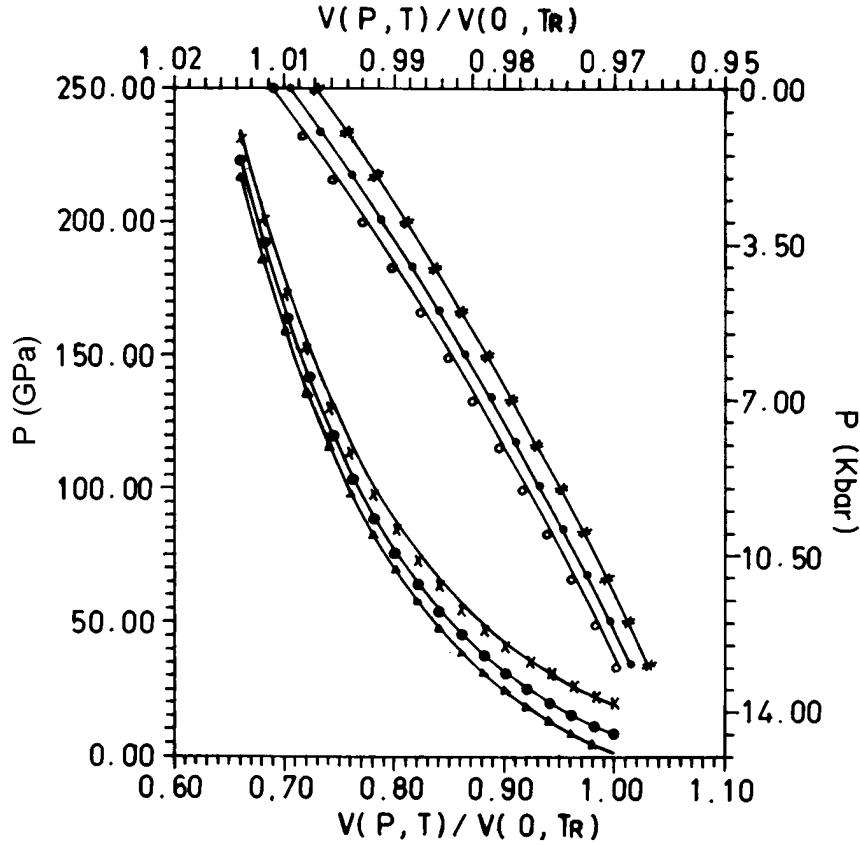
(c) The pressure dependence of the Grüneisen parameter  $\gamma(P, T)$  can be studied [12].

**Table 1.** Input data (10 kbar = 1 GPa).

Solids	Pressure range (kbar)	Temperature range (K)	$T_R$ (K)	$B_T(0, T_R)$ (kbar)	$B'_T(0, T_R)$	$Z$ ( $\times 10^{-4}$ kbar $^{-1}$ )	$\alpha(0, T_R)$ ( $\times 10^{-6}$ K $^{-1}$ )	RMSD at $T_R$
Au	0.0–2161.0	300.0–3000.0	300.0	1691.52	5.04	16.09	42.78 [17]	$1.54 \times 10^{-4}$
Mo	0.0–3000.0	293.0–7605.0	293.0	2709.02	3.58	0.84	15.00 [17]	$2.67 \times 10^{-3}$
W	0.0–3000.0	290.0–6905.0	293.0	3138.04	3.68	0.90	13.5 [17]	$4.05 \times 10^{-3}$
Hg	0.0–14.0	295.05–423.15	295.05	248.44	9.17	158.1	181.607 [15]	$2.04 \times 10^{-5}$

**Table 2.** Comparison of pressure (GPa) as a function of volume and temperature in Au:  $P_{exp}$ , experimental values taken from Heinz and Jeanolz [13];  $P_{calc}$ , our calculated values.

$V/V_0$	$T = 300$ K		$T = 500$ K		$T = 1000$ K		$T = 1500$ K		$T = 2000$ K		$T = 2500$ K		$T = 3000$ K	
	$P_{exp}$	$P_{calc}$	$P_{exp}$	$P_{calc}$	$P_{exp}$	$P_{calc}$	$P_{exp}$	$P_{calc}$	$P_{exp}$	$P_{calc}$	$P_{exp}$	$P_{calc}$	$P_{exp}$	$P_{calc}$
1.000	0.00	0.00	1.43	1.45	5.02	5.06	8.62	8.68	12.22	12.30	15.82	15.92	19.42	19.54
0.980	3.56	3.60	4.96	5.04	8.50	8.66	12.05	12.28	15.60	15.90	19.15	19.52	22.70	23.13
0.960	7.61	7.66	8.99	9.11	12.48	12.73	15.98	16.35	19.47	19.96	22.97	23.58	26.47	27.20
0.940	12.22	12.27	13.58	13.71	17.01	17.34	20.46	20.95	23.90	24.57	27.35	28.19	30.80	31.81
0.920	17.46	17.50	18.80	18.95	22.18	22.56	25.58	26.18	28.97	29.80	32.37	33.42	35.76	37.04
0.900	23.44	23.44	24.75	24.89	28.08	28.51	31.42	32.13	34.77	35.74	38.11	39.36	41.45	42.98
0.880	30.24	30.21	31.54	31.66	34.81	35.28	38.10	38.90	41.39	42.51	44.68	46.13	47.97	49.75
0.860	38.00	37.94	39.27	39.38	42.49	43.00	45.73	46.62	48.97	50.24	52.20	53.86	55.44	57.47
0.840	46.85	46.77	48.10	48.21	51.27	51.83	54.45	55.45	57.63	59.07	60.82	62.69	64.01	66.30
0.820	56.97	56.87	58.19	58.32	61.31	61.94	64.43	65.56	67.56	69.17	70.70	72.79	73.83	76.41
0.800	68.54	68.46	69.74	69.91	72.80	73.52	75.87	77.14	78.95	80.76	82.03	84.38	85.11	87.99
0.780	81.79	81.76	82.97	83.21	85.97	86.82	88.99	90.44	92.02	94.06	95.04	97.68	98.07	101.30
0.760	97.00	97.04	98.16	98.50	101.11	102.11	104.07	105.73	107.04	109.35	110.01	112.96	112.98	116.58
0.740	114.49	114.62	115.62	116.06	118.52	119.69	121.43	123.30	124.34	126.92	127.25	130.54	130.17	134.16
0.720	134.64	135.85	135.75	136.29	138.59	139.91	141.44	143.53	144.50	147.15	147.16	150.77	150.02	154.38
0.700	157.90	158.12	158.99	159.57	161.77	163.19	164.57	166.81	167.37	170.42	170.17	174.04	172.98	177.66
0.680	184.84	184.90	185.90	186.35	188.63	189.17	191.37	193.59	195.11	197.21	196.86	200.82	199.61	204.44
0.660	216.10	215.69	217.14	217.14	219.81	220.76	222.49	224.38	225.18	227.99	227.87	231.61	230.56	235.23



**Figure 1.** Pressure–volume relation of Au and Hg: —, present work; \*, experimental Hg data, 0–13 kbar, 21.9°C from [16]; ●, experimental Hg data, 0–13 kbar, 40.5°C, from [16]; ○, experimental Hg data, 0–13 kbar, 52.9°C, from [16]; △, experimental Au data, 0–250 GPa, 500 K from [15]; ⊙, experimental Au data, 0–250 GPa, 1000 K from [15]; ×, experimental Au data, 0–250 GPa, 1500 K, from [15].

Therefore, the parameter  $Z$  in the present theory is taken to be independent of both the pressure and the temperature. This assumption works very well and it is quite evident from the results reported later in tables 2 and 3.

(iv) The present EOS can also give the bulk modulus as a function of volume. For this purpose, we differentiate either equation (5) with respect to pressure or equation (8) with respect to volume at constant temperature and the result is

$$B_T(V, T) = \eta / \left\{ Z \left[ 1 + \beta \left( \frac{V(P, T)}{V(0, T_R)} \right)^\eta \right] \right\}. \quad (10)$$

(v) The Anderson–Grüneisen parameter  $\delta_T(P, T)$  is defined as

$$\delta_T(P, T) = - \frac{1}{\alpha(P, T) B_T(P, T)} \left( \frac{\partial B_T(P, T)}{\partial T} \right)_P. \quad (11)$$

Dass and Kumari [11] have obtained this parameter as

$$\delta_T(P, T) = B'_T(P, T) \quad (12)$$

**Table 3.** Comparison of density as a function of pressure and temperature for Mo and W.

<i>P</i> (GPa)	W				Mo	
	<i>T</i> (K)	$\rho$ (g cm <sup>-3</sup> )		<i>T</i> (K)	$\rho$ (g cm <sup>-3</sup> )	
		From [14]	Calculated		From [14]	Calculated
0.0	293.0	19.256	19.256	293.0	10.215	10.215
10.0	309.0	19.846	19.841	311.0	10.577	10.573
20.0	332.0	20.388	20.383	338.0	10.906	10.901
30.0	336.0	20.891	20.886	378.0	11.208	11.205
40.0	413.0	21.360	21.358	435.0	11.489	11.487
50.0	477.0	21.802	21.801	510.0	11.752	11.751
60.0	556.0	22.219	22.220	604.0	11.999	12.000
70.0	652.0	22.614	22.618	716.0	12.233	12.235
80.0	765.0	22.991	22.996	847.0	12.455	12.458
90.0	894.0	23.351	23.357	996.0	12.666	12.671
100.0	1040.0	23.695	23.702	1163.0	12.868	12.874
110.0	1202.0	24.026	24.033	1347.0	13.062	13.068
120.0	1380.0	24.345	24.352	1549.0	13.248	13.254
130.0	1573.0	24.652	24.659	1767.0	13.427	13.434
140.0	1582.0	24.948	24.956	2002.0	13.599	13.607
150.0	2006.0	25.235	25.243	2252.0	13.766	13.774
160.0	2244.0	25.513	25.521	2517.0	13.927	13.936
170.0	2496.0	25.782	25.790	2798.0	14.083	14.093
180.0	2762.0	26.044	26.052	3092.0	14.235	14.245
190.0	3042.0	26.298	26.307	3401.0	14.382	14.393
300.0	3334.0	26.546	26.555	3723.0	14.525	14.537
210.0	3639.0	26.787	26.797	4058.0	14.664	14.677
220.0	3957.0	27.022	27.032	4406.0	14.800	14.814
230.0	4286.0	27.251	27.263	4766.0	14.932	14.947
240.0	4628.0	27.475	27.488	5139.0	15.061	15.077
250.0	4980.0	27.693	27.708	5523.0	15.187	15.205
260.0	5344.0	27.907	27.924	5918.0	15.310	15.329
270.0	5719.0	28.116	28.135	6324.0	15.430	15.452
280.0	6104.0	28.320	28.342	6741.0	15.548	15.571
290.0	6499.0	28.521	28.545	7168.0	15.663	15.689
300.0	6905.0	28.717	28.744	7605.0	15.776	15.804

with the help of equation (9). On the other hand, Chang [13] has given this parameter as

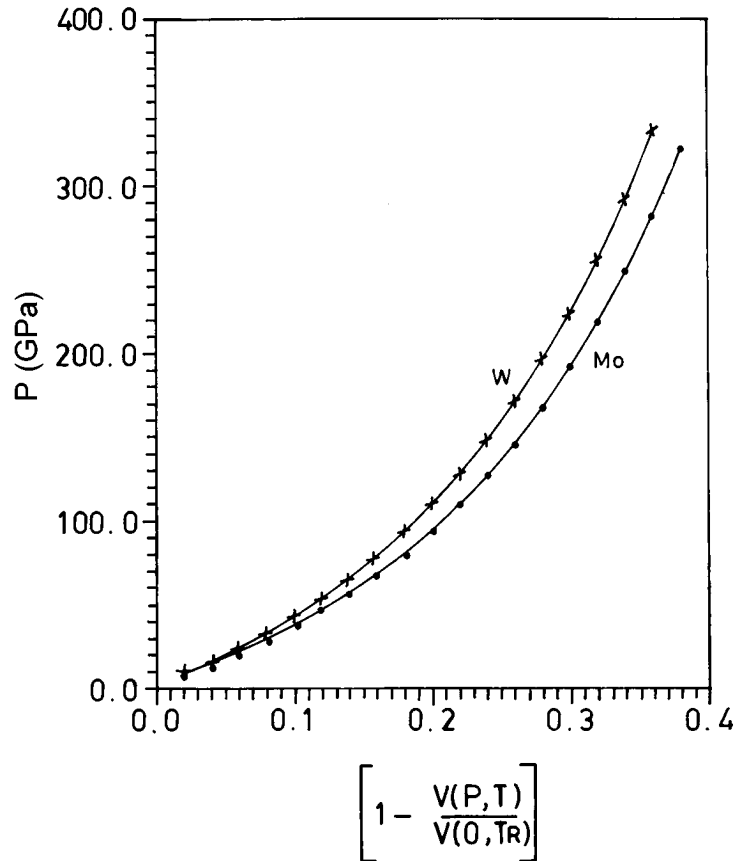
$$\delta_T(P, T) = B'_T(P, T) - 1. \quad (13)$$

The relation given by equation (12) is certainly better than that of equation (13) and has already been discussed elsewhere [4]. Thus, the variation in  $\delta_T(P, T)$  with pressure and temperature can be computed with the help of equation (7).

(vi) The present EOS can also be used to obtain a number of thermodynamic properties as a function of pressure. This will be discussed elsewhere.

### 3. Comparison with experiment

We shall be able to compare the predictions of equations (5)–(7) with the experimental data provided that the best fitted values of  $B_T(0, T_R)$ ,  $B'_T(0, T_T)$  and  $Z$  become available besides the value of  $\alpha(0, T_R)$ . The values of the first three parameters are obtained by the least-squares fitting technique for Au, Mo, W and Hg at a reference temperature  $T_R$ . The



**Figure 2.** Pressure–volume relation of Mo and W at 1000 K: —, present work; ×, W data, from [15], ●, Mo data, from [15].

values of these parameters together with other relevant data are reported in table 1. The experimental volume data are taken from Heinz and Jeanolz [14] for Au, from Hixson and Fritz [15] for Mo and W and from Davis and Gordon [16] for Hg.

### 3.1. Compression studies

By making use of equation (5) and taking the values of the relevant parameters from table 1, the volume is computed for Mo, W and Hg as a function of pressure at different temperatures. The pressure is calculated as a function of volume at different temperatures for Au.

The calculated values of  $P$  for Au are compared with the available data of Heinz and Jeanolz in table 1 and are plotted in figure 1. The agreement is very good as the discrepancy lies within  $\pm 3.5\%$  in the total ranges of pressures and temperatures.

The computation of density is done with the help of equation (5) for Mo and W. The results are compared with the Hugoniot results of Hixson and Fritz in table 3. The discrepancy is  $\pm 0.2\%$  for Mo and  $\pm 0.15\%$  for W in the total ranges of pressures and temperatures. Thus, very good agreement is observed here.



**Table 4.** Comparison of volume and  $B_T(0, T)$  as functions of pressure and temperature for liquid Hg. The results in parentheses are taken from Davis and Gordon [15].

$P$ (kbar)	$T = 21.09^\circ\text{C}$		$T = 40.5^\circ\text{C}$		$T = 52.9^\circ\text{C}$	
	$V(P, T)$ ( $V = 1$ at $0^\circ\text{C}$ )	$B_T(P, T)$ (kbar)	$V(P, T)$ ( $V = 1$ at $0^\circ\text{C}$ )	$B_T(P, T)$ (kbar)	$V(P, T)$ ( $V = 1$ at $0^\circ\text{C}$ )	$B_T(P, T)$ (kbar)
0.0	1.003 98 (1.003 98)	248.4 (248.4)	1.007 40 (1.007 36)	240.7 (243.1)	1.009 74 (1.009 62)	235.5 (239.6)
1.0	1.000 00 (1.000 00)	257.5 (257.6)	1.003 30 (1.003 30)	249.9 (252.4)	1.005 55 (1.005 51)	244.8 (248.9)
2.0	0.996 21 (0.996 21)	266.5 (266.6)	0.999 366 (0.999 410)	259.0 (261.3)	1.001 53 (1.001 56)	253.9 (257.9)
3.0	0.992 539 (0.992 540)	275.3 (275.3)	0.995 581 (0.995 650)	267.9 (270.1)	0.997 661 (0.997 74)	262.9 (266.7)
4.0	0.988 996 (0.988 00)	283.9 (284.0)	0.991 932 (0.992 030)	276.7 (278.7)	0.993 938 (0.994 060)	271.8 (275.4)
5.0	0.985 571 (0.985 570)	292.5 (292.5)	0.988 410 (0.988 530)	285.3 (287.3)	0.990 347 (0.990 510)	280.6 (283.9)
6.0	0.982 255 (0.982 250)	300.9 (300.8)	0.985 004 (0.985 140)	293.9 (295.6)	0.986 878 (0.997 070)	289.1 (292.3)
7.0	0.979 041 (0.979 040)	309.2 (309.1)	0.981 706 (0.981 860)	302.3 (303.9)	0.983 521 (0.983 730)	297.6 (300.5)
8.0	0.975 921 (0.975 900)	317.4 (317.0)	0.978 508 (0.978 600)	310.6 (312.0)	0.980 268 (0.980 510)	306.0 (309.0)
9.0	0.972 889 (0.972 900)	325.4 (325.0)	0.975 403 (0.975 600)	318.7 (320.0)	0.977 113 (0.977 380)	314.2 (317.0)
10.0	0.969 40 (0.969 900)	333.3 (333.0)	0.972 386 (0.972 600)	326.7 (328.0)	0.974 048 (0.974 340)	322.2 (325.0)
11.0	0.967 067 (0.967 100)	341.1 (341.0)	0.969 450 (0.969 700)	334.6 (336.0)	0.971 067 (0.971 380)	330.2 (333.0)
12.0	0.964 267 (0.964 300)	348.7 (349.0)	0.966 590 (0.966 800)	342.3 (344.0)	0.968 166 (0.968 510)	338.0 (341.0)
13.0	0.961 536 (0.961 500)	356.3 (357.0)	0.963 802 (0.964 000)	349.9 (352.0)	0.965 338 (0.965 720)	345.7 (348.0)

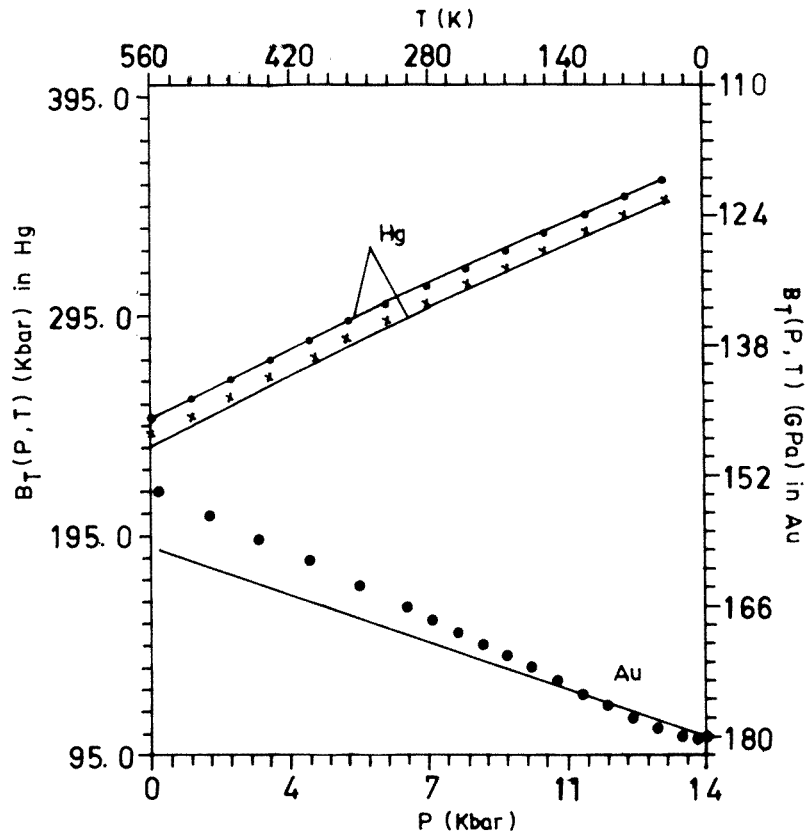
It is worthwhile to mention here that it is not possible to plot the data in table 3 because both  $P$  and  $T$  are varying. However,  $1 - V(P, T)/V(0, T_R)$  is plotted against  $P$  for Mo and W at 1000 K in figure 2 and the agreement is very good. The same is also true at other temperatures too.

The relative volume calculations are done for liquid Hg at 21.9, 40.5 and 52.9 °C up to 13 kbar pressure. The calculated results are compared with the data of Davis and Gordon in table 4 and are plotted in figure 1; they agree within  $\pm 0.05\%$  in the total ranges of pressures and temperatures.

Thus, it can be said from the above discussion that the present EOS is quite successful in representing the volume data as a function of pressure at different temperatures. This gives confidence in the use of the present EOS for high pressures and high temperatures.

### 3.2. Bulk modulus and its first derivative

The isothermal bulk modulus and its first pressure derivative as functions of pressure at different temperatures can be obtained from equations (6) and (7), respectively, after taking the values of the relevant parameters from table 1.



**Figure 3.** Variation in  $B_T(P, T)$  with  $P$  for Hg and with temperature for Au: —, present work; ●, experimental Hg data, 0–13 kbar, 21.9°C, from [16]; ×, experimental Hg data, 0–13 kbar, 52.9°C, from [16]; ●, experimental Au data,  $P = 0$ , 0–550 K, from [17].

Calculations for  $B_T(P, T)$  as a function of pressure at different temperatures are carried out for Hg. The calculated results are compared with the data of Davis and Gordon in table 4 and are plotted in figure 3. The agreement is very good.

For Au, equation (6) is used to compute the temperature dependence of the bulk modulus at  $P = 0$ . The calculated results are compared with the data given by Anderson *et al* [17] in table 5 and are plotted in figure 3. The agreement is fairly good. However, our results have a small temperature dependence.

No data are available for the bulk modulus as a function of pressure for Au, Mo and W. However, the calculations are done within the 0–400 kbar pressure range for each solid at 300 K with the help of equation (6) after making use of the relevant parameters from table 1. The results so obtained are plotted in figure 4. Furthermore, for completeness, we also report the temperature dependence of the bulk modulus for Mo and W in table 5 for ready reference.

As far as the calculations of  $B'_T(P, T)$  are concerned, no experimental or theoretical data are available for the materials studied here and hence no comparison is made. However, any one who is interested in this parameter can easily obtain the value at the desired pressure and temperature.

**Table 5.** Calculation of isothermal bulk modulus as a function of temperature for Au, Mo and W.

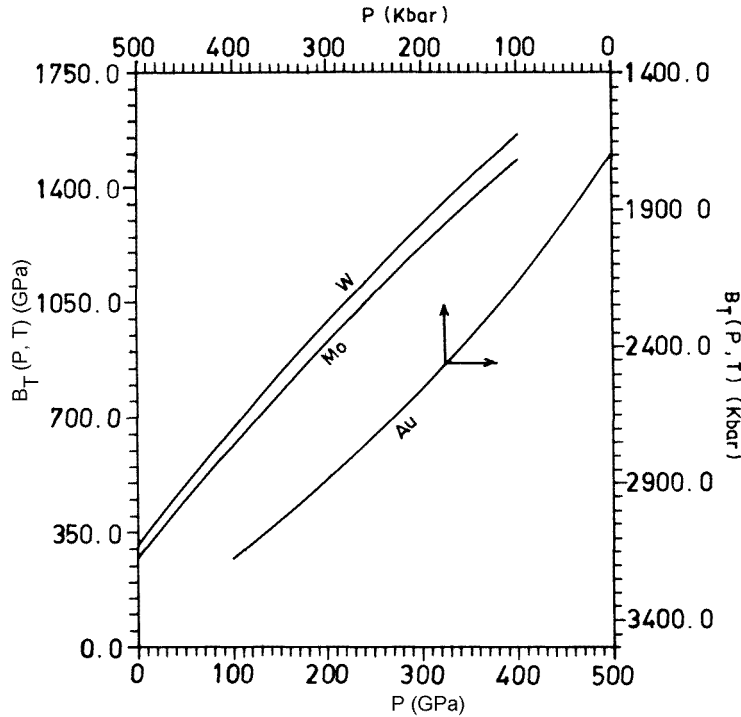
$T$ (K)	Au		$T$ (K)	Mo $B_T(0, T)$ , calculated (GPa)	W $B_T(0, T)$ , calculated (GPa)
	$B_T(0, T)$ , [17] (GPa)	$B_T(0, T)$ , calculated (GPa)			
0.0	180.32	180.07	25.0	274.80	317.98
10.0	180.32	179.71	50.0	274.43	317.59
25.0	180.13	179.17	75.0	274.07	317.20
50.0	179.33	178.26	100	273.00	316.81
75.0	178.09	177.35	150	272.98	316.09
100.0	176.73	176.44	200	272.25	315.25
125.0	175.41	175.53	300	270.80	313.69
150.0	174.07	174.62	400	269.34	312.13
175.0	172.81	173.71	500	267.89	310.57
200.0	171.53	172.80	600	266.43	309.01
225.0	170.24	171.88	700	264.97	307.45
250.0	168.99	170.98	800	263.52	305.89
275.0	167.76	170.06	900	262.06	304.33
300.0	166.51	169.15	1000	260.60	302.76
350.0	163.94	167.33	1200	257.68	299.64
400.0	161.22	165.50			
450.0	158.91	163.67			
500.0	156.49	161.84			
550.0	153.71	160.02			

**Table 6.** Comparison of  $\alpha(0, T)$  ( $\times 10^{-6} \text{ K}^{-1}$ ) as a function of temperature for Au, Mo and W;  $\alpha_{exp}(0, T)$  are the experimental values taken from [18];  $\alpha_{calc}$ , our calculated values.

$T$ (K)	Mo		W		Au	
	$\alpha_{exp}(0, T)$	$\alpha_{calc}(0, T)$	$\alpha_{exp}(0, T)$	$\alpha_{calc}(0, T)$	$\alpha_{exp}(0, T)$	$\alpha_{calc}(0, T)$
100	—	—	—	—	35.7	41.01
150	12.0	13.93	10.8	12.61	39.3	41.44
200	13.8	14.29	12.3	12.90	40.8	41.88
250	14.7	14.66	13.2	13.22	42.0	42.32
293	15.0	15.00	13.5	13.50	42.6	42.72
350	15.3	15.47	13.8	13.89	44.1	43.72
400	15.6	15.92	13.8	14.26	45.6	44.71
500	15.6	16.88	13.8	15.05	47.4	45.75
600	16.2	17.98	14.1	15.95	49.2	46.83
700	16.5	19.23	14.4	16.95	51.3	47.97
800	17.1	20.67	14.4	18.10	56.4	49.17
900	18.3	22.36	14.4	19.42	63.3	50.43

### 3.3. Thermal expansion

The calculations of  $\alpha(0, T)$  are done with the help of equation (9) for Au, Mo and W. The results are compared with the experimental data [18] for each solid in table 6. The overall agreement is good. However, the discrepancy increases with a rise in temperature.



**Figure 4.** Variation in  $B_T(P, T)$  with  $P$  for Au, Mo and W at 300 K: —, present work.

### 3.4. The Anderson–Grüneisen parameter

According to [4, 11], the Anderson–Grüneisen parameter is given by

$$\delta_T(P, T) = B'_T(P, T).$$

Thus, the variation in  $\delta_T(P, T)$  with pressure and temperature is the same as that of  $B'_T(P, T)$ , i.e.  $\delta_T(P, T)$  increases with rising temperature and decreases with increasing pressure.

### 4. Summary

The isothermal bulk modulus and its first pressure derivative, thermal expansion coefficient and the Anderson–Grüneisen parameter can be computed simultaneously together with volume compression as functions of pressure at different temperatures. The overall agreement between the calculated and the experimental value for various properties of Au, Mo, W and Hg is good. Thus, it appears that the present temperature-dependent EOS has great potential and scope as far as the practical applications in condensed matter are concerned.

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