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A new temperature-dependent equation of state of solids

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Abstract. In the present paper, a temperature-dependent equation of state (EOS) of solids is discussed which is found to be applicable in high-pressure and high-temperature range. Present equation of state has been applied in 18 solids. The calculated data are found in very good agreement with the data available from other sources.

Keywords. Temperature-dependent equation of state; solids; pressure and temperature.

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1. Introduction

The equation of state (EOS) of condensed matter is important in many fields of basic and applied sciences including physics and geophysics. To explain an EOS and other thermodynamical properties of a substance, it is essential to study the forces between atoms and molecules. The exact evaluation of these forces from atomic theory is one of the most difficult problems of quantum theory and wave mechanics. Due to lack of the precise knowledge of the interatomic forces, a theoretical EOS cannot easily be obtained. Therefore, to obtain an EOS, different simplifying models and approximations are being used and hence some empirical EOSs have been developed.

Semiempirical EOSs are based on some initial assumptions from either theoretical or experimental fact. For example, Murnaghan EOS is based on the empirical assumption that the isothermal bulk modulus is a linear function of pressure. Similarly, universal EOS is based on the universal relation between binding energy of the solids and intermolecular distance. In this direction, Kumari *et al* [1] have proposed a generalized form of an EOS, which is capable of reproducing some of the well-known EOSs available in literature. In the present paper, we have modified the basic assumption of Kumari *et al* [1] to obtain a new EOS.

2. Theory

To obtain the present EOS, we start with the assumption of Kumari *et al* [1], i.e.,

$$B'_{\mathrm{T}}(P, T_{\mathrm{R}}) = \left[\frac{\partial B(P, T_{\mathrm{R}})}{\partial P}\right]_{\mathrm{T}} = A\left[\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}\right]^{\xi} + C\left[\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}\right]^{-\eta}, \quad (1)$$

where A, C, ξ and η are pressure-independent parameters and T_{R} represents a reference or ambient temperature. By using the initial condition, $P = 0$, we get

$$V(P, T_{\mathrm{R}}) = V\,(0, T_{\mathrm{R}})$$

and

$$A + C = B'_{\mathrm{T}}(0, T_{\mathrm{R}}).$$

Now, putting

$$\left[\frac{\partial B_{\mathrm{T}}(P, T_{\mathrm{R}})}{\partial P}\right]_{\mathrm{T}} = -\frac{V(P, T_{\mathrm{R}})}{B_{\mathrm{T}}(P, T_{\mathrm{R}})}\left[\frac{\partial B_{\mathrm{T}}(P, T_{\mathrm{R}})}{\partial V(P, T_{\mathrm{R}})}\right]_{\mathrm{T}}$$

and integrating eq. (1), we obtain

$$\frac{B_{\mathrm{T}}(P, T_{\mathrm{R}})}{B_{\mathrm{T}}(0, T_{\mathrm{R}})} = \exp\left[-\frac{A}{\xi}\left\{\left(\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}\right)^{\xi} - 1\right\} + \frac{C}{\eta}\left\{\left(\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}\right)^{-\eta} - 1\right\}\right]. \quad (2)$$

But eq. (2) cannot be further exactly integrated to obtain the expression for $V(P, T_{\mathrm{R}})/V(0, T_{\mathrm{R}})$ as a function of pressure and hence some approximation is required. Further, four parameters are involved.

Therefore, to obtain an exact EOS, we have modified eq. (1) as

$$B_{\mathrm{T}}(P, T_{\mathrm{R}})\left[\frac{\partial B_{\mathrm{T}}(P, T_{\mathrm{R}})}{\partial P}\right]_{\mathrm{T}} = A\left[\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}\right]^{-\alpha}, \quad (3)$$

where A and α are constants in the sense that these parameters have values at initial condition, i.e. $P = 0$ and $T = T_{\mathrm{R}}$. Thus, by changing the initial condition, the values of these parameters will also change. Once the initial condition is imposed, the values of these parameters become independent of pressure and temperature.

Equation (3) can be rewritten as

$$B_{\mathrm{T}}(P, T_{\mathrm{R}})\left[\frac{\partial B_{\mathrm{T}}(P, T_{\mathrm{R}})}{\partial V}\right]_{\mathrm{T}}\left[\frac{\partial V(P, T_{\mathrm{R}})}{\partial P}\right]_{\mathrm{T}}\left[\frac{-V(P, T_{\mathrm{R}})}{-V(P, T_{\mathrm{R}})}\right] = A\left[\frac{V\,(P, T_{\mathrm{R}})}{V\,(0, T_{\mathrm{R}})}\right]^{-\alpha}$$

or

$$\mathrm{d}B_{\mathrm{T}}(P, T_{\mathrm{R}}) = A\left[\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}\right]^{-\alpha}\left(-\frac{\mathrm{d}V}{V}\right). \quad (4)$$

To obtain eq. (4), we have used

$$-\frac{1}{V(P,T_{\rm R})}\left[\frac{{\rm d}V(P,T_{\rm R})}{{\rm d}P}\right]_{\rm T}=\frac{1}{B_{\rm T}(P,T_{\rm R})}.$$

Integrating eq. (4) in the limit $P=0$ and $T=T_{\rm R}$, we get

$$B_{\rm T}(P,T_{\rm R})=B_{\rm T}(0,T_{\rm R})+\frac{A}{\alpha}\left[\left\{\frac{V(P,T_{\rm R})}{V(0,T_{\rm R})}\right\}^{-\alpha}-1\right]. \tag{5}$$

Now, using the definition of bulk modulus as stated above, eq. (5) can be transformed to

$$\begin{aligned}-\,{\rm d}P\;=\;&B_{\rm T}(0,T_{\rm R})\left[\frac{\partial V(P,T_{\rm R})}{V(P,T_{\rm R})}\right]+\frac{A}{\alpha}\left\{\frac{V(P,T_{\rm R})}{V(0,T_{\rm R})}\right\}^{-\alpha}\left[\frac{\partial V(P,T_{\rm R})}{V(P,T_{\rm R})}\right]\\&-\frac{A}{\alpha}\left[\frac{\partial V(P,T_{\rm R})}{V(P,T_{\rm R})}\right].\end{aligned} \tag{6}$$

Integrating eq. (6) in the limit $P=P$ and $P=0$, we get

$$P=\left[-B_{\rm T}(0,T_{\rm R})+\frac{A}{\alpha}\right]\ln\left(\frac{V(P,T_{\rm R})}{V(0,T_{\rm R})}\right)+\frac{A}{\alpha^2}\left[\left(\frac{V(P,T_{\rm R})}{V(0,T_{\rm R})}\right)^{-\alpha}-1\right]. \tag{7}$$

Equation (7) represents the new generalized three-parameter isothermal EOS. Here, $B_{\rm T}(0,T_{\rm R})$, A and α are pressure- and temperature-independent adjustable parameters.

Using the limiting case $P=0$ and representing the first pressure derivative of the bulk modulus at ambient temperature $B'_{\rm T}(0,T_{\rm R})$ in eq. (3), we get

$$B_{\rm T}(0,T_{\rm R})B'_{\rm T}(0,T_{\rm R})=A. \tag{8}$$

Differentiation of eq. (3) with pressure gives

$$\left[B'_{\rm T}(P,T_{\rm R})\right]^2+B_{\rm T}(P,T_{\rm R})B''_{\rm T}(P,T_{\rm R})=\frac{A\alpha}{B_{\rm T}(P,T_{\rm R})}\frac{[V(P,T_{\rm R})]^{-\alpha}}{[V(0,T_{\rm R})]^{-\alpha}}. \tag{9}$$

Using the limiting case $P=0$ in eq. (9), we have

$$\left[B'_{\rm T}(0,T_{\rm R})\right]^2+B_{\rm T}(0,T_{\rm R})B''_{\rm T}(0,T_{\rm R})=\frac{A\alpha}{B_{\rm T}\,(0,T_{\rm R})}.$$

Putting the value of A from eq. (8), we get

$$\left[B'_{\rm T}(0,T_{\rm R})\right]^2+B_{\rm T}(0,T_{\rm R})B''_{\rm T}(0,T_{\rm R})=B'_{\rm T}\,(0,T_{\rm R})\alpha. \tag{10}$$

2.1 *Murnaghan EOS*

Since the value of the second pressure derivative of the bulk modulus, i.e. the value of $B''_{\rm T}\,(P,T_{\rm R})$ is very small, to a good approximation $B''_{\rm T}\,(P,T_{\rm R})=0$ can be taken. Thus, we get

$$\alpha=B'_{\rm T}(0,T_{\rm R}). \tag{11}$$

Now substituting the value of A from eq. (8) and the value of α from eq. (11) in eq. (7), we get

$$\frac{V(P,T_{\mathrm{R}})}{V(0,T_{\mathrm{R}})}=\left[1+\frac{B'_{\mathrm{T}}(0,T_{\mathrm{R}})}{B_{\mathrm{T}}(0,T_{\mathrm{R}})}P\right]^{-1/B'_{\mathrm{T}}(0,T_{\mathrm{R}})}. \tag{12}$$

This is the well-known Murnaghan equation of state.

Further, taking logarithm of eq. (12) on both sides and using that if $x<1$, then $\ln x = x-1$, it will give Tait-like equation of state where x represents the LHS term of eq. (12).

It is a well accepted view that lesser the adjustable parameters in an EOS, better is the EOS.

We have seen that if $B''_{\mathrm{T}}(0,T_{\mathrm{R}})=0$, α becomes equal to $B'_{\mathrm{T}}(0,T_{\mathrm{R}})$ and eq. (7) converts to the well-known Murnaghan EOS which is not valid at high pressures [2]. Therefore, we are in search of a new EOS, which can also be valid at high pressures.

2.2 *Present EOS*

It is a well accepted view that lesser the adjustable parameters in an EOS, better is the EOS. Thus, we have to reduce the parameters from three to two and for this purpose, we take the following approach.

The value of $B''_{\mathrm{T}}(0,T_{\mathrm{R}})$ is always negative but small. Therefore, α has to be less than $B'_{\mathrm{T}}(0,T_{\mathrm{R}})$. Hence, we take $\alpha=(3/4)B'_{\mathrm{T}}(0,T_{\mathrm{R}})$ in the present EOS to give very good agreement with the experimental data and now the present EOS has only two adjustable parameters as given below:

$$\begin{aligned}P =& \frac{B_{\mathrm{T}}(0,T_{\mathrm{R}})}{3}\ln\left[\frac{V(P,T_{\mathrm{R}})}{V(0,T_{\mathrm{R}})}\right]\\ &+\frac{16}{9}\frac{B_{\mathrm{T}}(0,T_{\mathrm{R}})}{B'_{\mathrm{T}}(0,T_{\mathrm{R}})}\left[\left(\frac{V(P,T_{\mathrm{R}})}{V(0,T_{\mathrm{R}})}\right)^{-(3/4)B'_{\mathrm{T}}(0,T_{\mathrm{R}})}-1\right].\end{aligned} \tag{13}$$

2.3 *Temperature-dependent EOS*

We can introduce the thermal effect into the isothermal EOS to convert it into temperature-dependent EOS through the approximation that the thermal pressure is independent of the volume and is linear with temperature, provided that temperature $T\geq(\Theta/2)$ [3–5] where Θ is the Debye temperature. Mathematically, it is expressed as

$$P_{\mathrm{th}}=B_{\mathrm{T}}(0,T_{\mathrm{R}})\alpha(0,T_{\mathrm{R}})\,(T-T_{\mathrm{R}})\,. \tag{14}$$

The involved parameters of EOS in the present approach are $B_{\mathrm{T}}(0,T_{\mathrm{R}})$, $B'_{\mathrm{T}}(0,T_{\mathrm{R}})$ and $\alpha(0,T_{\mathrm{R}})$, where $\alpha(0,T_{\mathrm{R}})$ is the thermal expansion coefficient at zero pressure and at ambient temperature, T_{R}. Moreover, this approach not only predicts the P–V variation at different temperatures other than reference temperature, but also helps in calculating the temperature dependence of thermal expansion, $\alpha(P,T)$, isothermal bulk modulus, $B(P,T)$ and its first pressure derivative, $B'_{\mathrm{T}}(P,T)$.

To include the thermal effect in an isothermal EOS, the pressure at any other temperature T will be written as

$$P(T) = P(T_{\mathrm{R}}) + P_{\mathrm{th}}$$

or

$$P(T) = P(T_{\mathrm{R}}) + \alpha(0, T_{\mathrm{R}}) B_{\mathrm{T}}(0, T_{\mathrm{R}})\,(T - T_{\mathrm{R}})\,. \tag{15}$$

Table 1. Input parameters along with root mean square deviation (RMSD) used in temperature-dependent EOS.

Substance	Pressure range (kbar)	Temperature range (K)	T_{R} (K)	$B_{\mathrm{T}}(0, T_{\mathrm{R}})$ (kbar)	$B'_{\mathrm{T}}(0, T_{\mathrm{R}})$	$\alpha(0, T_{\mathrm{R}}) \times 10^{-5}$ K^{-1}	RMSD at T_{R}	Ref. (exp. data)
Au	0–2161	300–3000	300	1692.7 1670.0 [18]	5.309 5.500 [18]	4.278 [9]	1.315	[18]
W	0–3000	293–1000	293	3130.1 3138.0 [6]	3.827 3.680 [6]	1.35 [9]	3.442	[19]
Mo	0–3000	293–1000	293	2694.70 2703.70 [6]	3.772 3.722 [6]	1.50 [9]	0.693	[19]
NaCl	0–309.29	298–1073	298	244.55 240.14 [26]	4.636 4.540 [26]	11.91[22]	0.416	[20]
CsCl	0–432.32	298–1073	298	177.720 172.51 [26]	5.110 4.960 [26]	13.84 [22]	0.708	[20]
Cu	0–2400	293–6653	293	1290.00 1298.50 [23]	5.260 5.186 [23]	5.01 [22]	5.567	[21]
Tantalum	0–2300	293–7374	293	1963.40 1989.00 [24]	3.499 3.581 [24]	1.95 [22]	1.435	[21]
Tungsten carbide	0–2000	293–2176	293	3619.90 3637.00 [25]	4.319 4.500 [25]	1.32 [22]	1.243	[21]
Stainless steel	0–1900	293–4091	293	1592.9	4.993	4.77 [22]	2.807	[21]
Iridium	0–3000	293–5635	293	3400.70 3401.30 [23]	4.808 4.764 [23]	1.95 [22]	1.468	[21]
Platinum	0–2700	293–6193	293	2732.60 2737.59 [23]	5.0914 4.968 [23]	2.67 [22]	1.753	[21]
2024-Al	0–1200	293–4684	293	765.43 798.00 [25]	4.173 4.500 [25]	6.54 [22]	2.211	[21]
Palladium	0–2100	293–5239	293	1785.50	5.554	3.48 [22]	3.296	[21]
Niobium	0–1800	293–5369	293	1708.90 1676 [24]	3.598 4.034 [24]	2.13 [22]	1.379	[21]
Chromium	0–1400	293–2160	293	1867.50 1869.20 [23]	5.191 5.075 [23]	1.50 [22]	2.065	[21]
Hafnium	0–600	293–1310	293	1131.40 1122.50 [23]	3.351 3.424 [23]	1.80 [22]	0.312	[21]
Vanadium	0–1300	293–2568	293	1563.90 1589.60 [24]	3.695 3.585 [24]	2.34 [22]	1.147	[21]
Beryllium	0–900	293–1330	293	1177.8 1200.00 [24]	3.355 3.469 [24]	3.36 [22]	1.822	[21]

Equation (14) has been used extensively by other workers in literature [6–8]. Substitution of eq. (15) into eq. (13) gives

$$P(T) = \frac{B_{\mathrm{T}}(0, T_{\mathrm{R}})}{3} \ln\left[\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}\right] + \frac{16}{9}\frac{B_{\mathrm{T}}(0, T_{\mathrm{R}})}{B'_{\mathrm{T}}(0, T_{\mathrm{R}})}\left[\left(\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}\right)^{-(3/4)B'_{\mathrm{T}}(0,T_{\mathrm{R}})} - 1\right] + \alpha(0, T_{\mathrm{R}})B_{\mathrm{T}}(0, T_{\mathrm{R}})\,(T - T_{\mathrm{R}})\,. \tag{16}$$

Equation (16) represents a new temperature-dependent EOS and $\alpha(0, T_{\mathrm{R}})$ is the thermal expansion coefficient. Present EOS is capable of giving some important results.

(1) *Product of* $\alpha(P, T)$ *and* $B_{\mathrm{T}}(P, T)$ *is a constant*

Differentiating eq. (16) with respect to temperature at constant volume, we have

$$\left[\frac{\partial P}{\partial T}\right]_{\mathrm{V}} = \alpha(0, T_{\mathrm{R}})B_{\mathrm{T}}(0, T_{\mathrm{R}})$$

Table 2. Comparison of pressure with volume compression $V(P, T_{\mathrm{R}})/V(0, T_{\mathrm{R}})$ in NaCl using the experimental data [29].

$\frac{V(P, T_{\mathrm{R}})}{V(0, T_{\mathrm{R}})}$	P (kbar) (Expt.)	P (kbar) (Calc.) Tait EOS	P (kbar) (Calc.) B-MEOS	P (kbar) (Calc.) Present EOS
0.883	40	40.5119	40.6494	40.6215
0.819	78	76.9541	77.7988	77.7099
0.810	84	83.2160	84.2626	84.1634
0.796	95	93.6104	95.0510	94.9365
0.788	102	99.9289	101.6462	101.5236
0.778	110	108.2384	110.3637	110.2326
0.751	137	133.1602	136.8255	136.6854
0.731	161	154.2260	159.5813	159.4589
0.722	170	164.5085	170.8234	170.7196
0.713	183	175.3260	182.7482	182.6720
0.708	190	181.5771	189.6856	189.6292
0.705	194	185.4132	193.9599	193.9171
0.701	200	190.6299	199.7934	199.7710
0.699	202	193.2827	202.7691	202.7580
0.698	204	194.6204	204.2720	204.2667
0.687	222	209.8431	221.4884	221.5606
0.680	232	220.0334	233.1311	233.2666
0.679	235	221.5222	234.8402	234.9857
0.672	247	232.1825	247.1371	247.3606
0.660	268	251.4647	269.6503	270.0429
0.658	272	254.8071	273.5886	274.0144
0.650	288	268.5600	289.9057	290.4803
0.649	290	270.3231	292.0107	292.6059
0.645	300	277.4758	300.5813	301.2634

whereas thermodynamic identity gives

$$\left[\frac{\partial P}{\partial T}\right]_{\mathrm{V}} = \alpha(P,T)B_{\mathrm{T}}(P,T).$$

Hence

$$\left[\frac{\partial P}{\partial T}\right]_{\mathrm{V}} = \alpha(0,T_{\mathrm{R}})B_{\mathrm{T}}(0,T_{\mathrm{R}}) = \alpha(P,T)B_{\mathrm{T}}(P,T) = \xi. \tag{17}$$

Here ξ is a pressure- and temperature-independent parameter. Equation (17) gives the same result which has already been used by Kumari and Dass [9] for wide application in condensed matter [10–14].

Table 3. Comparison of pressure as a function of $\rho(P,T)$ at different temperatures with Hugoniot shock wave data in molybdenum and tungsten.

Molybdenum (Mo)				Tungsten (W)			
$\rho(P,T)$ (g/cm^3)	T (K)	P (Expt.) (kbar)	P (Calc.) (kbar)	$\rho(P,T)$ (g/cm^3)	T (K)	P (Expt.) (kbar)	P (Calc.) (kbar)
10.577	311.00	100.00	100.94	19.846	309.00	100.00	100.76
10.906	338.00	200.00	201.39	20.388	332.00	200.00	201.11
11.208	378.00	300.00	301.26	20.891	366.00	300.00	301.25
11.489	435.00	400.00	401.13	21.360	413.00	400.00	400.95
11.752	510.00	500.00	500.94	21.802	477.00	500.00	500.85
11.999	604.00	600.00	600.49	22.219	556.00	600.00	600.48
12.233	716.00	700.00	700.13	22.614	652.00	700.00	699.91
12.455	847.00	800.00	799.67	22.991	765.00	800.00	799.53
12.666	996.00	900.00	898.92	23.351	894.00	900.00	899.07
12.868	1163.00	1000.00	998.29	23.695	1040.00	1000.00	998.39
13.062	1347.00	1100.00	1097.80	24.026	1202.00	1100.00	1097.90
13.248	1549.00	1200.00	1197.20	24.345	1380.00	1200.00	1197.50
13.427	1767.00	1300.00	1296.50	24.652	1573.00	1300.00	1297.00
13.599	2002.00	1400.00	1395.50	24.948	1782.00	1400.00	1396.40
13.766	2252.00	1500.00	1494.90	25.235	2006.00	1500.00	1495.90
13.927	2517.00	1600.00	1593.90	25.513	2244.00	1600.00	1595.50
14.083	2798.00	1700.00	1693.00	25.782	2496.00	1700.00	1694.90
14.235	3092.00	1800.00	1792.40	26.044	2762.00	1800.00	1794.50
14.382	3401.00	1900.00	1891.40	26.298	3042.00	1900.00	1893.90
14.525	3723.00	2000.00	1990.40	26.546	3334.00	2000.00	1993.60
14.664	4058.00	2100.00	2089.30	26.787	3639.00	2100.00	2093.10
14.800	4406.00	2200.00	2188.50	27.022	3957.00	2200.00	2192.60
14.932	4766.00	2300.00	2287.30	27.251	4286.00	2300.00	2292.00
15.061	5139.00	2400.00	2386.30	27.475	4628.00	2400.00	2391.60
15.187	5523.00	2500.00	2485.10	27.693	4980.00	2500.00	2490.80
15.310	5918.00	2600.00	2583.90	27.907	5344.00	2600.00	2590.30
15.430	6324.00	2700.00	2682.40	28.116	5719.00	2700.00	2689.60
15.548	6741.00	2800.00	2781.30	28.320	6104.00	2800.00	2788.70
15.663	7168.00	2900.00	2879.70	28.521	6499.00	2900.00	2888.30
15.776	7605.00	3000.00	2978.40	28.717	6905.00	3000.00	2987.40

(2) *Relation for* $\alpha(P,T)$ *in terms of* $B_{\mathrm{T}}(P,T)$

Applying the thermal effect into eq. (13), we get

$$\begin{aligned} P(T) = {} & \frac{B_{\mathrm{T}}(0,T_{\mathrm{R}})}{3}\ln\left[\frac{V(P,T_{\mathrm{R}})}{V(0,T_{\mathrm{R}})}\right] \\ & +\frac{16}{9}\frac{B_{\mathrm{T}}(0,T_{\mathrm{R}})}{B'_{\mathrm{T}}(0,T_{\mathrm{R}})}\left[\left(\frac{V(P,T_{\mathrm{R}})}{V(0,T_{\mathrm{R}})}\right)^{-(3/4)B'_{\mathrm{T}}(0,T_{\mathrm{R}})}-1\right]+\xi(T-T_{\mathrm{R}}). \end{aligned}$$

Equation (17) can now be written as

$$\alpha(P,T)=\frac{\alpha(0,T_{\mathrm{R}})B_{\mathrm{T}}(0,T_{\mathrm{R}})}{B_{\mathrm{T}}(P,T)}. \qquad (18)$$

Hence eq. (18) gives the temperature and pressure variation of $\alpha(P,T)$.

Table 4. Comparison of pressure as a function of $\rho(P,T)$ at different temperatures with Hugoniot shock wave data in copper and tantalum.

Copper (Cu)				Tantalum (Ta)			
$\rho(P,T)$ (g/cm^3)	T (K)	P (Expt.) (kbar)	P (Calc.) (kbar)	$\rho(P,T)$ (g/cm^3)	T (K)	P (Expt.) (kbar)	P (Calc.) (kbar)
9.499	336.00	100.00	96.53	17.457	319.00	100.00	101.40
9.959	395.00	200.00	194.10	18.170	361.00	200.00	201.84
10.349	479.00	300.00	292.71	18.815	427.00	300.00	301.74
10.688	589.00	400.00	391.73	19.407	522.00	400.00	401.48
10.990	726.00	500.00	491.53	19.956	648.00	500.00	501.25
11.262	888.00	600.00	591.61	20.468	804.00	600.00	600.88
11.510	1072.00	700.00	691.85	20.949	992.00	700.00	700.61
11.738	1279.00	800.00	792.26	21.403	1209.00	800.00	800.33
11.949	1505.00	900.00	892.56	21.834	1455.00	900.00	900.22
12.145	1751.00	1000.00	992.64	22.244	1728.00	1000.00	1000.10
12.329	2014.00	1100.00	1092.80	22.636	2029.00	1100.00	1100.20
12.502	2294.00	1200.00	1192.90	23.011	2355.00	1200.00	1200.30
12.666	2589.00	1300.00	1293.10	23.371	2706.00	1300.00	1300.50
12.820	2900.00	1400.00	1392.50	23.718	3081.00	1400.00	1401.00
12.967	3224.00	1500.00	1492.00	24.052	3478.00	1500.00	1501.40
13.107	3561.00	1600.00	1591.40	24.375	3897.00	1600.00	1602.00
13.241	3910.00	1700.00	1690.70	24.687	4337.00	1700.00	1702.50
13.368	4271.00	1800.00	1789.10	24.989	4797.00	1800.00	1803.10
13.491	4643.00	1900.00	1887.90	25.282	5277.00	1900.00	1903.80
13.608	5026.00	2000.00	1985.90	25.567	5775.00	2000.00	2004.60
13.721	5419.00	2100.00	2083.90	25.843	6291.00	2100.00	2105.20
13.829	5821.00	2200.00	2181.10	26.113	6824.00	2200.00	2206.20
13.934	6232.00	2300.00	2278.60	26.375	7374.00	2300.00	2307.00
14.035	6653.00	2400.00	2375.60				

(3) *Derivation for Anderson–Grüneisen parameter*

By differentiating eq. (18) with pressure at constant temperature, we get

$$\left[\frac{\partial B_{\mathrm{T}}(P,T)}{\partial P}\right]_{\mathrm{T}} = \frac{-B_{\mathrm{T}}(P,T)}{\alpha(P,T)}\left[\frac{\partial \alpha(P,T)}{\partial P}\right]_{\mathrm{T}}. \tag{19}$$

Using the thermodynamic identity

$$\left[\frac{\partial \alpha(P,T)}{\partial P}\right]_{\mathrm{T}} = \frac{1}{[B_{\mathrm{T}}(P,T)]^2}\left[\frac{\partial B_{\mathrm{T}}(P,T)}{\partial T}\right]_{\mathrm{P}}$$

and substituting in eq. (19), we get

$$\left[\frac{\partial B_{\mathrm{T}}(P,T)}{\partial P}\right]_{\mathrm{T}} = -\frac{1}{\alpha(P,T)B_{\mathrm{T}}(P,T)}\left[\frac{\partial B_{\mathrm{T}}(P,T)}{\partial T}\right]_{\mathrm{P}}. \tag{20}$$

On the other hand, Anderson–Grüneisen parameter [15] is given as

$$\delta_{\mathrm{T}}(P,T) = -\frac{1}{\alpha(P,T)B_{\mathrm{T}}(P,T)}\left[\frac{\partial B_{\mathrm{T}}(P,T)}{\partial T}\right]_{\mathrm{P}}.$$

Thus, we get the following important result:

$$B'_{\mathrm{T}}(P,T) = \delta_{\mathrm{T}}(P,T). \tag{21}$$

This result is the same as the one reported for the first time by Dass and Kumari [12].

Table 5. Comparison of pressure as a function of $\rho(P,T)$ at different temperatures with Hugoniot shock wave data in tungsten carbide and stainless steel.

Tungsten carbide				Stainless steel			
$\rho(P,T)$ (g/cm^3)	T (K)	P (Expt.) (kbar)	P (Calc.) (kbar)	$\rho(P,T)$ (g/cm^3)	T (K)	P (Expt.) (kbar)	P (Calc.) (kbar)
15.415	305.00	100.00	99.96	8.326	332.00	100.00	99.39
15.780	322.00	200.00	200.17	8.684	382.00	200.00	198.96
16.118	345.00	300.00	299.94	8.992	452.00	300.00	298.68
16.435	377.00	400.00	399.91	9.264	544.00	400.00	398.79
16.733	419.00	500.00	499.78	9.507	659.00	500.00	498.82
17.015	471.00	600.00	599.70	9.728	795.00	600.00	599.11
17.283	533.00	700.00	699.69	9.931	951.00	700.00	699.62
17.538	604.00	800.00	799.48	10.118	1127.00	800.00	799.93
17.781	685.00	900.00	898.95	10.293	1322.00	900.00	900.84
18.015	776.00	1000.00	998.87	10.456	1534.00	1000.00	1001.40
18.238	876.00	1100.00	1098.00	10.609	1763.00	1100.00	1101.80
18.454	986.00	1200.00	1197.60	10.753	2007.00	1200.00	1201.90
18.661	1104.00	1300.00	1296.60	10.890	2266.00	1300.00	1302.40
18.862	1232.00	1400.00	1396.10	11.019	2540.00	1400.00	1402.20
19.055	1368.00	1500.00	1494.80	11.143	2826.00	1500.00	1502.60
19.243	1513.00	1600.00	1593.90	11.260	3125.00	1600.00	1601.90
19.424	1667.00	1700.00	1692.40	11.373	3436.00	1700.00	1701.90
19.601	1828.00	1800.00	1791.30	11.481	3758.00	1800.00	1801.40
19.772	1998.00	1900.00	1889.70	11.585	4091.00	1900.00	1901.10
19.939	2176.00	2000.00	1988.30				

(4) $\alpha(0, T)$ *as a function of temperature*

Differentiating eq. (17) with temperature, keeping pressure constant, we have

$$\left[\frac{\partial\alpha(P,T)}{\partial T}\right]_{\mathrm{P}} B_{\mathrm{T}}(P,T) + \alpha(P,T)\left[\frac{\partial B_{\mathrm{T}}(P,T)}{\partial T}\right] = 0,$$

$$\frac{1}{[\alpha(P,T)]^2}\left[\frac{\partial\alpha(P,T)}{\partial T}\right]_{\mathrm{P}} = \delta_{\mathrm{T}}(P,T) = B'_{\mathrm{T}}(P,T)\,. \tag{22}$$

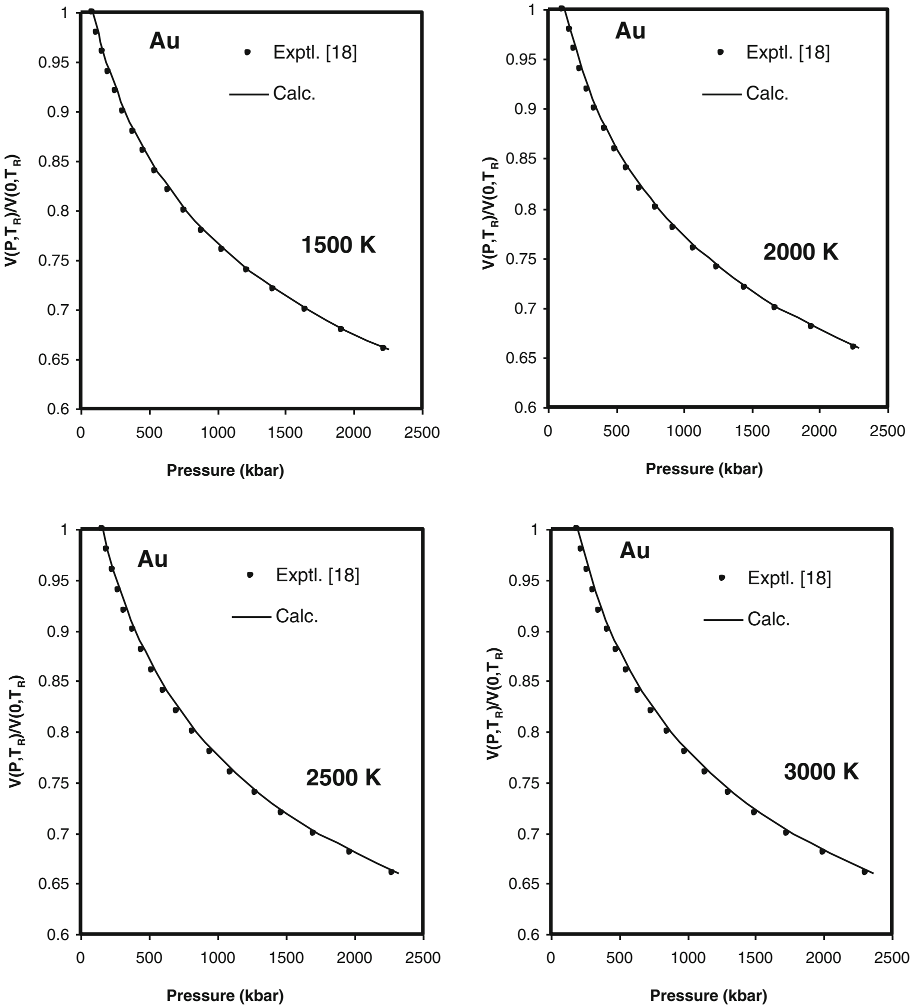

Figure 1. Variation of volume compression $V(P,T_{\mathrm{R}})/V(0,T_{\mathrm{R}})$ with pressure for Au at different temperatures.

Taking $P = 0$, eq. (22) can easily be integrated for the temperature limit $T = T$ and $T = T_{\mathrm{R}}$ to give the result as

$$\alpha\,(0, T) = \frac{\alpha\,(0, T_{\mathrm{R}})}{1 - B'_{\mathrm{T}}\,(0, T_{\mathrm{R}})\alpha(0, T_{\mathrm{R}})\,(T - T_{\mathrm{R}})}. \tag{23}$$

The same result has been obtained by many others [9,16,17].

3. Calculations and discussion

Isothermal EOS given by eq. (13) has been applied in 18 solids including NaCl by using best fitted values of $B_{\mathrm{T}}(0, T_{\mathrm{R}})$ and $B'_{\mathrm{T}}(0, T_{\mathrm{R}})$ at reference temperature. The best fitted values of $B_{\mathrm{T}}(0, T_{\mathrm{R}})$ and $B'_{\mathrm{T}}(0, T_{\mathrm{R}})$ along with the root mean square deviation (RMSD) are

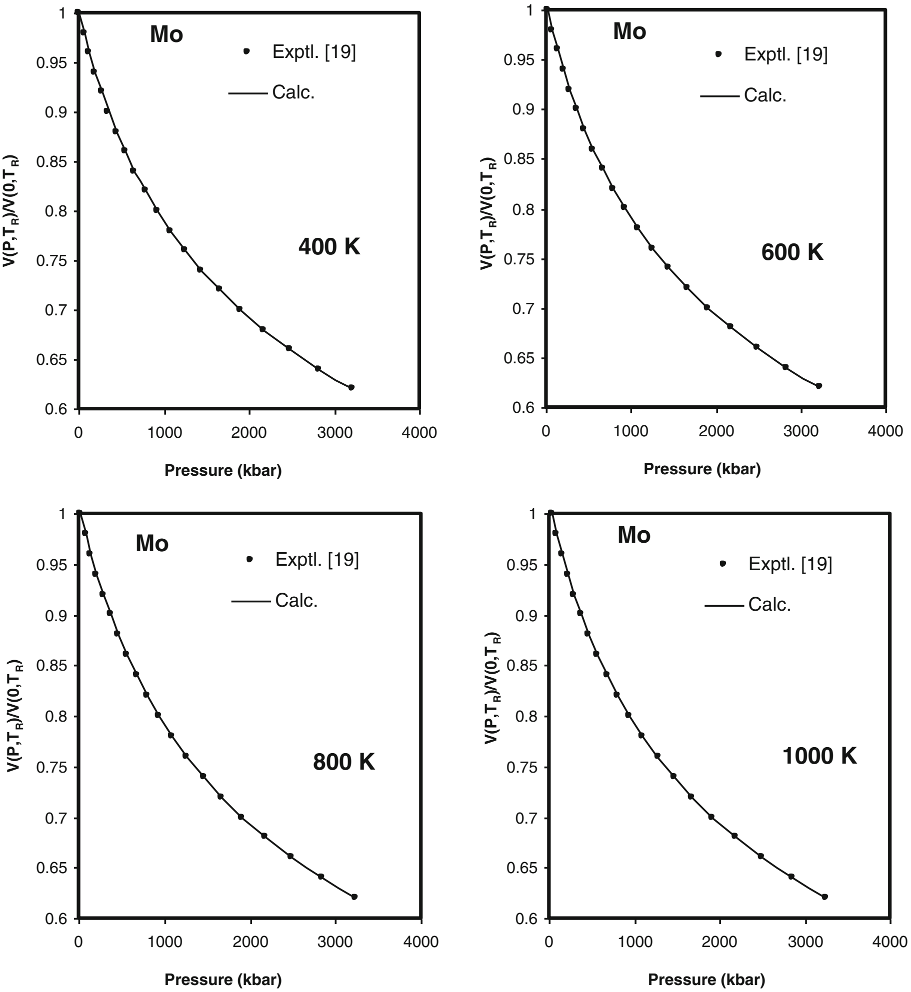

Figure 2. Variation of volume compression $V(P, T_{\mathrm{R}})/V(0, T_{\mathrm{R}})$ with pressure for Mo at different temperatures.

reported in table 1. Table 1 also contains the values of $B_T(0, T_R)$ and $B'_T(0, T_R)$ given by other workers just for comparison. It is clearly evident from table 1 that the present EOS is quite successful in representing the isothermal EOS.

Further, to show the validity of the present EOS given by eq. (13), we have computed pressure P by using the input values of $V(P, T_R)/V(0, T_R)$ in the case of NaCl and have compared our results with that given by Tait EOS [27] and by Birch-Murnaghan EOS [28] along with experimental data of Liu *et al* [29] in table 2. It is evident from table 2 that present EOS is as good as Birch-Murnaghan EOS and better than Tait EOS.

Using temperature-dependent EOS given by eq. (16) and taking the values of the relevant parameters from table 1, the pressure has been computed for 18 solids at different temperatures and the computed values are compared with the experimental data in tables 3, 4 and 5 in the case of molybdenum, tungsten, copper, tantalum, tungsten carbide and stainless steel as a function of $\rho(P, T)$. The agreement in each solid is very good. Further, the calculated and the experimental pressure data along with $V(P, T_R)/V(0, T_R)$ are plotted in the case of gold and molybdenum in figures 1 and 2 at four different temperatures. The references of the data used in the present EOS are reported in table 1. From the reported data and the plots it is clear that the calculated values are in very good agreement with the experimental data.

4. Conclusion

From the results shown in tables and graphs, it can be concluded that the present EOS is capable of representing the volume/density data of the solids successfully in the high-pressure and high-temperature range. Further, other thermodynamical properties like $B_T(P, T)$, $\alpha(P, T)$ and $\delta(P, T)$ may also be computed as a function of temperature and pressure. The computations of these parameters are not done because the computation is simple and no experimental data are available for comparison.

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