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Pressure dependence of Gruneisen parameter of some transition metals

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ABSTRACT

Comparison of seismic velocities in mantle metals under mantle conditions with seismic data is the first step towards constraining mantle chemistry. The calculation, however, is uncertain due to lack of data on certain physical properties. The Grüneisen parameter (γ) is of much importance regarding to the physical properties of mantle metals, because it sets limitations on the thermo elastic properties of the lower mantle and core at different compression ratio.The Grüneisen parameter of ten transition metals; Mo, Cd, Co, Zn, La, Cu, Ag, Au, Fe and Hf have been calculated using three equation of states viz; Brennan Stacey EOS, Shanker EOS and Vinet EOS, taking isothermal bulk modulus and its first pressure derivative into the consideration. On the basis of calculations it is concluded that, except for Hf, the Shanker EOS is the best for calculating Gruneisen parameter at both high and low compression ranges for transition metals, where as Vinet EOS is applicable at high compression ratio.

Key words: Gruneisen parameter,Anderson Gruneisen Parameter, EOS, transition metals, isothermal bulk modulus

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INTRODUCTION

In the reduction of shock-wave data to isothermal data, the knowledge of pressure dependence of the Gruneisen parameter is very useful. The volume variation of Gruneisen parameter (γ) is very important in theoretical equation of state, geophysical models, ultrasonic measurements and

melting of solids. The Grüneisen parameter has considerable appeal to geophysicists because it is an approximately constant, dimensionless parameter that varies slowly as a function of pressure and temperature. It has both a microscopic and macroscopic definition, the former relating it to the vibrational frequencies of atoms in a material, and the latter relating it to familiar Classical thermodynamic properties such as heat capacity and thermal expansion. Unfortunately, the experimental determination of Grüneisen parameter (γ), defined in either way, is extremely difficult; the macroscopic definition requires a detailed knowledge of the phonon dispersion spectrum of the material, whereas the microscopic definition requires experimental measurements of thermodynamic properties at high pressure and temperature. As a result of the difficulty associated with obtaining experimentally an accurate value for Grüneisen parameter (γ), [a number of more approximate expressions have been suggested by Poirire [1]] many of these relate to Grüneisen parameter (γ) at atmospheric pressure (P=0) to the first derivative of the bulk modulus with respect to pressure K_T' via γ = (1/2)K_T'–X, where X is constant. These relations may be expanded to take into account the variation of Grüneisen parameter (γ) with pressure. In these more general cases, Grüneisen parameter γ (P) is a function of the equation of state. Despite the intrinsic relationship between Grüneisen parameter (γ) and equation of state [2], it is frequently the case that the choice of the functional form of both the Grüneisen parameter and the equation of state to which it should be related are made independently of each other, and somewhat arbitrarily; this has resulted in a literature in which there is a wide range of value of Grüneisen parameter (γ) for many geologically relevant materials. It is therefore, important to investigate more carefully how the value of Grüneisen parameter (γ) and its compressional behaviour are affected by:

(1) the choice of the formulation of Grüneisen parameter (γ)
(2) the use of different equation of state.

At first we will review the various formulations of Grüneisen parameter (γ), starting from how they may be obtained directly from the equation of state. In the present work the Grüneisen parameter has been estimated at different compression for ten transition metals; Mo, Cd, Co, Zn, La, Cu, Ag, Au, Fe, Hf using three phenomenological isothermal equations of state viz; Brennan Stacey EOS, Shanker EOS and Vinet EOS.

The Grüneisen Parameter

Stacey assumed that the correlation of motions along a bond was the same with respect to dilation as that of those transverse to the bond. Thus, Borton and Stacey [3], find correlation for Grüneisen parameter (γ) with leading relevant parameters, using equation

$$\gamma_{ba-s} = \frac{\left(\frac{1}{2}\right)K_T' - \frac{1}{6} - \frac{f}{3}\left[1 - \frac{1}{3}\left(\frac{P}{K_T}\right)\right]}{1 - \left(\frac{4}{3}\right)\left(\frac{P}{K_T}\right)} \qquad (1)$$

where f=2.35 and K_T & K_T' are isothermal bulk modulus and its first pressure derivative respectively.

At P=0, equation (1) reduces to

$$\gamma_{ba-s} = \frac{1}{2}K_0^{'} - 0.95 \qquad (2)$$

Computation of Grüneisen parameter (γ) From Equation of State

The three phenomenological forms of isothermal equation of state as derived from lattice potential theory [4] are as follows:

$$P = \frac{3K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{(3K_0^{'}-5)}\left[\exp\left\{\left(\frac{3K_0^{'}-5}{3}\right)\times\left(1-\frac{V}{V_0}\right)\right\}-1\right] \qquad (3)$$

$$P = \frac{3K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{(3K_0^{'}-8)}\left[\left(1-\frac{1}{t}+\frac{2}{t^2}\right)(\exp(ty)-1)+y\left(1+y-\frac{2}{t}\right)\exp(ty)\right] \qquad (4)$$

where y = (1-V/V_0) and t = ($K_0^{'}$-8/3)

$$P = 3K_0 x^{-2}(1-x)\exp[\eta(1-x)] \qquad (5)$$

where x=(V/V_0)$^{1/3}$ and η=(3/2)($K_0^{'}$-1)

V is the volume at pressure P and V_0 is the volume at zero pressure, K_0 and $K_0^{'}$ are the isothermal bulk modulus and its first pressure derivative at zero pressure respectively. Equation (3) is the Brennan-Stacey EOS derived, using the thermodynamic formulation for the Grüneisen parameter [5,6]. Equation (4) is the Shanker EOS derived using a modified exponential dependence for the short range force constant on volume [7]. Equation (5) is the Vinet EOS based on universal relationship between binding energy and interatomic separation for solids [8, 9]

Expression for isothermal bulk modulus corresponding to equations (3), (4), and (5) obtained using the relationship $K_T = -V(dP/dV)_T$ are given as follows:

$$K_T = K_0\left(\frac{V}{V_0}\right)^{-\frac{1}{3}}\exp\left\{\left(K_0^{'}-\frac{5}{3}\right)\left(1-\frac{V}{V_0}\right)\right\}+\frac{4}{3}P \qquad (6)$$

$$K_T = K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}} \exp\left\{\left(K_0^{'} - \frac{8}{3}\right)\left(1 - \frac{V}{V_0}\right)\right\} + \frac{4}{3}P \qquad (7)$$

$$K_T = K_0 x^{-2}[1 + (\eta x + 1)(1 - x)]\exp\{\eta(1 - x)\} \qquad (8)$$

The corresponding expression for $K_T^{'}$ = (dK_T/dP) obtained from equations (6), (7), and (8) are written as follows:

$$K_T^{'} = \left(1 - \frac{4}{3}\frac{P}{K_T}\right)\left\{\left(K_0^{'} - \frac{5}{3}\right)\frac{V}{V_0} + \frac{5}{3}\right\} + \frac{16}{9}\frac{P}{K_T} \qquad (9)$$

$$K_T^{'} = \left(1 - \frac{4}{3}\frac{P}{K_T}\right)\left\{\left(K_0^{'} - \frac{8}{3}\right)\frac{V}{V_0} + \frac{8}{3}\right\} + \frac{16}{9}\frac{P}{K_T} \qquad (10)$$

$$K_T^{'} = \frac{1}{3}\left[\frac{x(1 - \eta) + 2\eta x^2}{1 + (\eta x + 1)(1 - x)} + \eta x + 2\right] \qquad (11)$$

Thus equations (3), (6), and (9) represent the Brennan Stacey EOS, equations (4), (7), and (10) represent the Shanker EOS and equations (5), (7), and (11), represent the Vinet EOS.

Anderson-Grüneisen Parameter

The physical significance of the Anderson-Grüneisen Parameter (δ_T) has been emphasized by several workers. Boehler *et al.* [10] and Chopelas [11] demonstrated that Anderson-Grüneisen parameter (δ_T) is independent of volume (V) upto the certain compression limit in their experiments. Chopelas and Boehler [12] have also shown the validity of this assumption. Duffy and Ahrens [13] found consistency in their interpretation of shock data under the assumption that Anderson-Grüneisen parameter (δ_T) is constant along a Hugoniot.

Anderson [14] has shown that the thermal expansivity of a crystal under the effect of pressure can be studied by analyzing the volume at different pressure. The parameter is defined as

$$\delta_T(P, T) = \left(\frac{1}{\alpha(P, T)K_T(P, T,)}\right)\left(\frac{\partial K_T(P, T)}{\partial T}\right)_P \qquad (12)$$

$\alpha(P,T)$ is the coefficient of thermal expansivity.

On the basis of Grüneisen relation Chang [15] expressed Anderson-Grüneisen parameter (δ_T) as

$$\delta_T(P, T) = \left[\frac{\partial K_T(P, T)}{\partial P}\right]_T - 1 \qquad (13)$$

a more generalised form of this equation is suggested by Dass and Kumari[16], according to which Anderson-Grüneisen parameter (δ_T) expressed as

$$\delta_T(P,T) = \left[\frac{\partial K_T(P,T)}{\partial P}\right]_T = K_T' \qquad (14)$$

RESULTS AND DISCUSSION

In the present work we have described three different forms of EOS; equations (3), (4), and (5). Equation (3) corresponds to Brennan-Stacey EOS, equation (4) corresponds to Shanker EOS and equation (5) corresponds to Vinet EOS. All the three EOS contains only two parameters K_0 and K_0' both at zero pressure. It has been the usual practice to adjust or to fit the parameters K_0 and K_0' in order to achieve the agreement with the experimental values. This procedure of fitting does not provides a useful insight for the physical EOS. In order to make a real test of EOS we have used experimental values of K_0 and K_0' for given elements. These values of K_0 and K_0' have been recommended by Anderson [17]. The values of pressure P for ten different transition metals viz. Mo, Cd, Co, Zn, La, Cu, Ag, Au, Fe and Hf ; were computed for given increments of V/V_0 by using equation (3), (4) and (5). The value of input parameter, K_0 and K_0' are taken from literature [17, 18]. Using the value of pressure P computed from equations (3), (4) and (5) for ten different transition metal elements, the values of first pressure derivative of bulk modulus (K_T) at constant temperature are computed from equations (6), (7) and (8). Substituting these values P and K_T, in equations (9), (10) and (11) the value of K_T' was obtained. Substituting the value of K_T' in equation (14) we get the value of Anderson Grüneisen Parameter (δ_T). Further substituting the values of P, K_T and K_T', in equation (1) the value of $\gamma_{ba\text{-}s}$ were calculated. A graph is plotted between the Grüneisen parameter (γ) versus V/V_0, leads to the following generalization.

The graphs plotted between Grüneisen parameter (γ) versus V/V_0 which are obtained by Brennan-Stacey EOS and Shanker EOS, are straight line for most of the elements except hafnium, but it is a curved for the values obtained by Vinet EOS. It has been noted that, for a good approximation the ratio γ/Ω (where $\Omega=V/V_0$) of Grüneisen parameter to volume is constant for solids [19]. Fang and Rong [20] have calculated the melting temperature under high pressure with the assumption that γ/Ω is constant, has been frequently used in work on shock compression of metals.

The expression γ/Ω leads to equation of straight line ($y=mx+c$). Hence the graph between Grüneisen parameter (γ) versus Ω must be a straight line which strongly supports the Brennan-Stacey EOS and Shanker EOS both under low and high compressions where as Vinet equation is applicable only at high compression ratio. Thus, Brennan-Stacey and Shanker EOS is compatible both low and high compression ranges for calculating Grüneisen parameter whereas Vinet EOS

is incompatible for calculating the Grüneisen parameter using equation (18) at low compression ranges.

Input value of Bulk modulus (K_0) and its first pressure derivative (K_0') for ten different transition elements at zero pressure which we have used in our calculations is given in Table-1

Table – 1: Input value of Bulk modulus (K_0) and its first pressure derivative (K_0') for different elements at zero pressure

S.No	Element	K_0	K_0'
1	**Molubdenum**	**253.10**	**13.29**
2	**Cadmium**	**47.30**	**4.08**
3	**Cobalt**	**167.10**	**17.33**
4	**Zinc**	**61.46**	**3.26**
5	**Lanthanum**	**24.62**	**2.86**
6	**Copper**	**151.03**	**4.01**
7	**Silver**	**110.73**	**4.62**
8	**Gold**	**166.40**	**4.55**
9	**Iron**	**171.11**	**7.79**
10	**Hafnium**	**108.95**	**0.59**

In spite of this reservation on Grüneisen parameter (γ) the evidence supports the idea that the exponential variation of Grüneisen parameter (γ) with volume is much different at high pressure in comparison to low pressure. This conclusion is also supported by the work of Kopyshev [21], who investigated the behaviour of Grüneisen parameter (γ) using Fermi-Dirac theory. He found that Grüneisen parameter (γ) approached the limiting value of 1/2 at a condition of vanishing volume. This conclusion also agrees with the results of Rice [22], by assuming that both the adiabatic bulk modulus and Grüneisen parameter (γ) are independent of temperature. He found that

$$\frac{\gamma}{V} = \frac{\gamma_0}{V_0}\left[1+\gamma_0\left(1-\frac{V}{V_0}\right)\right]^{-2}$$

Using a harmonic theory, Pastine [23] computed the curve for Grüneisen parameter (γ) versus V, which shows smaller exponent at higher pressure.

It is not always necessary to make a prior assumption of the volume dependence of Grüneisen parameter (γ) in order to compute temperature effect in shock waves. Another way tried by Takeuchi and Kanamori [24] makes an assumption about thermal equation of state, and the empirical relationship γ vs V/V_0. For example, Takeuchi and Kanamori [24] assumed that the γ vs V/V_0 curve is linear and that the pressure-energy relationship is given by one of the Mie-Grüneisen equation. It is interesting to note that the values of Grüneisen parameter (γ) computed by their method indicates that the exponential power of V for Grüneisen parameter (γ) is higher at low pressure than at high pressure. Such evidences strongly support that Grüneisen parameter

Table – 2: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Molubdenum using (a) Brennan- Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	K_T' (a)=δ_T	K_T' (b)=δ_T	K_T' (c)=δ_T	$\gamma_{ba\text{-}s}$ (a)	$\gamma_{ba\text{-}s}$ (b)	$\gamma_{ba\text{-}s}$ (c)
1.00	0.00	0.00	0.00	253.10	253.10	253.10	13.29	13.29	7.94	5.81	5.81	5.81
0.90	55.06	55.17	53.10	911.43	916.08	845.63	11.26	11.35	5.58	5.23	5.28	3.44
0.80	270.36	272.63	236.72	3146.68	3214.94	2529.88	9.86	10.05	4.25	4.65	4.75	2.26
0.70	1109.67	1131.00	852.30	10791.72	11363.17	7468.04	8.64	8.94	3.38	4.07	4.22	1.55
0.60	4451.31	4598.54	2994.48	37273.29	41142.44	22891.02	7.48	7.89	2.76	3.49	3.69	1.07
0.50	18266.15	19148	11143.15	130812	154670	76058.75	6.33	6.88	2.29	2.91	3.16	0.72
0.40	78788.76	83773	47078.83	471647	614677	288440.96	5.21	5.90	1.91	2.32	2.62	0.45
0.30	369859	398261	247982.04	1783003	2666097	1352667.04	4.10	4.95	1.58	1.74	2.09	0.21
0.20	2030584	2209197	1942046.91	7427499	13549880	9184326.57	3.02	4.04	13.29	1.16	1.56	0.00

Table – 3: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Cadmium using (a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	K_T' (a)=δ_T	K_T' (b)=δ_T	K_T' (c)=δ_T	$\gamma_{ba\text{-}s}$ (a)	$\gamma_{ba\text{-}s}$ (b)	$\gamma_{ba\text{-}s}$ (c)
1.00	0.00	0.00	0.00	47.30	47.30	47.30	4.08	4.08	4.08	1.21	1.21	1.21
0.90	6.16	6.17	6.16	70.60	70.95	70.75	3.55	3.64	3.41	1.09	1.14	1.01
0.80	16.38	16.48	16.44	104.46	106.53	105.48	3.13	3.29	2.90	0.97	1.07	0.82
0.70	33.53	33.96	33.89	154.70	161.69	158.44	2.77	3.01	2.51	0.85	1.00	0.66
0.60	63.01	64.37	64.43	231.45	250.55	242.41	2.47	2.77	2.19	0.72	0.92	0.50
0.50	115.80	119.45	120.65	353.89	401.27	382.78	2.20	2.56	1.92	0.60	0.85	0.34
0.40	216.69	225.80	232.37	562.57	676.52	635.68	1.97	2.39	1.69	0.48	0.78	0.18
0.30	431.57	454.25	482.81	958.93	1240.48	1146.01	1.76	2.23	1.48	0.36	0.71	0.00
0.20	989.32	1051.22	1175.25	1878.09	2657.48	2394.74	1.58	2.10	1.28	0.24	0.64	-0.25

Table – 4: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Cobalt using (a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	K_T' (a)=δ_T	K_T' (b)=δ_T	K_T' (c)=δ_T	$\gamma_{ba\text{-}s}$ (a)	$\gamma_{ba\text{-}s}$ (b)	$\gamma_{ba\text{-}s}$ (c)
1.00	0.00	0.00	0.00	167.10	167.10	167.10	17.33	17.33	17.33	7.83	7.83	5.17
0.90	46.51	46.61	43.21	890.62	895.20	772.39	14.76	14.85	9.21	4.09	7.10	3.19
0.80	314.96	317.88	241.29	4545.85	4646.34	3031.01	13.01	13.20	6.18	2.55	6.36	2.14
0.70	1866.79	1906.21	1109.73	23141.39	24398.23	11713.66	11.41	11.72	4.59	1.70	5.63	1.49
0.60	11056.68	11452.88	5104.60	118831.1	131558.67	47716.34	9.86	10.29	3.59	1.15	4.90	1.04
0.50	67604.29	71085.16	25674.5	619702.4	737173.0	216397.0	8.31	8.88	2.90	0.77	4.17	0.70
0.40	435957.22	464961.06	153115.1	3312397.2	4367125.4	1165932.9	6.77	7.51	2.39	0.47	3.43	0.43
0.30	3063211.77	3307658.64	1213063.8	18475807.1	28232277.2	8256861.7	5.25	6.17	1.97	0.23	2.70	0.20
0.20	25182043.0	27460764.2	15863454.4	112448180.6	213811999	93756345.3	3.76	4.87	1.62	0.02	1.97	-0.01

Table – 5: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Zinc using (a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	K_T' (a)=δ_T	K_T' (b)=δ_T	K_T' (c)=δ_T	$\gamma_{ba\text{-}s}$ (a)	$\gamma_{ba\text{-}s}$ (b)	$\gamma_{ba\text{-}s}$ (c)
1.00	0.00	0.00	0.00	61.46	61.46	61.46	3.26	3.26	3.26	0.80	0.80	0.80
0.90	7.67	7.68	5.34	84.91	85.32	85.08	2.89	2.98	2.83	0.72	0.77	0.68
0.80	19.50	19.61	15.08	117.12	119.41	118.05	2.59	2.75	2.48	0.64	0.74	0.57
0.70	38.06	38.53	33.03	162.52	169.66	165.42	2.33	2.55	2.19	0.56	0.71	0.46
0.60	68.01	69.39	67.19	228.72	246.74	235.98	2.11	2.39	1.95	0.48	0.68	0.34
0.50	118.53	122.01	135.69	330.15	371.45	346.44	1.92	2.25	1.74	0.40	0.65	0.22
0.40	209.86	218.00	284.92	497.32	589.09	531.80	1.76	2.13	1.55	0.32	0.62	0.07
0.30	394.50	413.54	655.72	806.85	1016.28	877.42	1.62	2.03	1.38	0.24	0.59	-0.11
0.20	851.68	900.47	1814.98	1512.75	2048.01	1648.65	1.50	1.93	1.21	0.16	0.56	-0.41

Table – 6: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Lanthanum using (a) Brennan Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	K_T' (a)=δ_T	K_T' (b)=δ_T	K_T' (c)=δ_T	γ_{ba-s} (a)	γ_{ba-s} (b)	γ_{ba-s} (c)
1.00	0.00	0.00	0.00	24.62	24.62	24.62	2.86	2.86	2.86	0.60	0.60	0.60
0.90	3.01	3.01	3.01	32.75	32.91	32.79	2.57	2.66	2.53	0.54	0.59	0.51
0.80	7.49	7.53	7.51	43.67	44.52	43.89	2.33	2.49	2.25	0.48	0.58	0.43
0.70	14.29	14.47	14.36	58.75	61.30	59.38	2.12	2.34	2.02	0.42	0.57	0.34
0.60	24.95	25.44	25.18	80.37	86.54	81.77	1.95	2.22	1.82	0.36	0.56	0.24
0.50	42.45	43.65	43.04	113.02	126.63	115.72	1.80	2.11	1.64	0.30	0.55	0.13
0.40	73.30	76.03	74.70	166.23	195.34	170.79	1.67	2.01	1.47	0.24	0.54	0.00
0.30	134.27	140.45	137.21	263.98	327.90	269.66	1.56	1.93	1.32	0.18	0.53	-0.19
0.20	282.20	297.59	286.08	485.89	643.05	480.87	1.46	1.86	1.17	0.12	0.52	-0.57

Table – 7: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter (γ_{ba-s}) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Copper using (a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	K_T' (a)=δ_T	K_T' (b)=δ_T	K_T' (c)=δ_T	γ_{ba-s} (a)	γ_{ba-s} (b)	γ_{ba-s} (c)
1.00	0.00	0.00	0.00	151.03	151.03	151.03	4.01	4.01	4.01	1.17	1.17	1.17
0.90	19.59	19.62	19.60	223.85	224.96	224.36	3.49	3.58	3.36	1.05	1.10	0.98
0.80	51.89	52.20	52.09	329.14	335.65	332.37	3.08	3.24	2.87	0.94	1.04	0.80
0.70	105.75	107.11	106.87	484.56	506.41	496.21	2.73	2.97	2.48	0.82	0.97	0.64
0.60	197.81	202.06	202.20	720.93	780.18	754.56	2.44	2.73	2.17	0.70	0.90	0.48
0.50	361.74	373.07	376.61	1096.44	1242.40	1183.91	2.18	2.54	1.91	0.59	0.84	0.33
0.40	673.46	701.58	720.83	1734.18	2082.77	1952.53	1.95	2.36	1.68	0.47	0.77	0.17
0.30	1334.0	1403.67	1486.68	2942.16	3797.39	3492.52	1.74	2.21	1.47	0.35	0.70	-0.01
0.20	3041.0	3229.93	3585.52	5738.21	8088.77	7229.46	1.57	2.08	1.27	0.23	0.63	-0.26

Table – 8: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Silver using (a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	K_T' (a)=δ_T	K_T' (b)=δ_T	K_T' (c)=δ_T	$\gamma_{ba\text{-}s}$ (a)	$\gamma_{ba\text{-}s}$ (b)	$\gamma_{ba\text{-}s}$ (c)
1.00	0.00	0.00	0.00	110.73	110.73	110.73	4.62	4.62	4.62	1.48	1.48	1.48
0.90	14.82	14.85	14.83	173.83	174.69	174.10	3.76	4.07	3.76	1.33	1.38	1.20
0.80	40.64	40.89	40.77	269.43	274.80	271.65	3.15	3.65	3.15	1.18	1.28	0.97
0.70	85.96	87.11	86.79	416.90	436.06	426.39	2.69	3.31	2.69	1.03	1.18	0.76
0.60	167.27	171.02	171.00	650.50	705.61	681.98	2.32	3.03	2.32	0.89	1.09	0.58
0.50	318.98	329.48	333.27	1035.52	1179.54	1128.10	2.02	2.78	2.02	0.74	0.99	0.40
0.40	620.67	648.01	671.86	1710.55	2075.52	1970.38	1.76	2.57	1.76	0.59	0.89	0.22
0.30	1287.67	1358.75	1473.50	3022.41	3972.66	3761.42	1.53	2.38	1.53	0.44	0.79	0.04
0.20	3080.21	3282.59	3838.87	6114.44	8886.90	8422.77	1.31	2.21	1.31	0.30	0.70	-0.19

Table – 9: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Gold using (a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	K_T' (a)=δ_T	K_T' (b)=δ_T	K_T' (c)=δ_T	$\gamma_{ba\text{-}s}$ (a)	$\gamma_{ba\text{-}s}$ (b)	$\gamma_{ba\text{-}s}$ (c)
1.00	0.00	0.00	0.00	166.40	166.40	166.40	6.51	6.51	6.51	2.42	2.42	2.42
0.90	24.64	24.68	24.58	312.58	314.14	311.01	5.53	5.62	4.91	2.18	2.23	1.83
0.80	75.61	76.12	75.09	573.03	584.77	566.27	4.80	4.98	3.90	1.94	2.04	1.39
0.70	181.08	183.77	179.26	1042.79	1093.09	1031.34	4.19	4.46	3.21	1.70	1.85	1.05
0.60	403.28	413.51	400.74	1906.94	2081.05	1917.95	3.66	4.01	2.69	1.45	1.65	0.77
0.50	888.64	922.00	899.41	3546.49	4094.14	3719.75	3.17	3.61	2.29	1.21	1.46	0.54
0.40	2014.78	2116.39	2130.90	6815.52	8487.16	7734.58	2.71	3.25	1.96	0.97	1.27	0.33
0.30	4905.65	5215.17	5658.12	13917.35	19163.73	18026.70	2.28	2.92	1.67	0.73	1.08	0.12
0.20	13854.92	14889.16	18742.72	32178.56	50643.23	51491.87	1.89	2.61	1.41	0.48	0.88	-0.09

Table – 10: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Iron using (a) Brennan-Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	$K_T'(a)=\delta_T$	$K_T'(b)=\delta_T$	$K_T'(c)=\delta_T$	$\gamma_{ba\text{-}s}$ (a)	$\gamma_{ba\text{-}s}$ (b)	$\gamma_{ba\text{-}s}$ (c)
1.00	0.00	0.00	0.00	171.11	171.11	171.11	7.79	7.79	7.79	3.06	3.06	3.06
0.90	27.16	27.21	27.01	363.12	364.94	358.38	6.59	6.69	5.59	2.76	2.81	2.20
0.80	90.41	91.05	88.60	747.67	763.21	720.74	5.72	5.90	4.32	2.45	2.55	1.62
0.70	237.24	240.97	228.57	1525.74	1601.24	1444.77	4.99	5.27	3.48	2.14	2.29	1.19
0.60	584.09	599.94	556.46	3127.24	3423.62	2963.38	4.34	4.71	2.88	1.84	2.04	0.86
0.50	1433.34	1491.04	1373.94	6514.39	7572.10	6379.67	3.73	4.21	2.42	1.53	1.78	0.60
0.40	3640.10	3836.54	3630.58	14000.06	17664.78	14888.70	3.15	3.74	2.05	1.22	1.52	0.36
0.30	9970.97	10640.80	10970.35	31863.91	44925.18	39647.84	2.60	3.30	1.74	0.92	1.27	0.15
0.20	31782.04	34290.68	42745.84	81584.71	133808.81	133421.80	2.08	2.89	1.46	0.61	1.01	-0.06

Table - 11: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for Hafnium using (a) Brennan Stacey EOS (b) Shanker EOS (c) Vinet EOS at $T=T_0=300K$

V/V_0	P(a)	P(b)	P(c)	K_T(a)	K_T(b)	K_T(c)	$K_T'(a)=\delta_T$	$K_T'(b)=\delta_T$	$K_T'(c)=\delta_T$	$\gamma_{ba\text{-}s}$ (a)	$\gamma_{ba\text{-}s}$ (b)	$\gamma_{ba\text{-}s}$ (c)
1.00	0.00	0.00	0.00	108.95	108.95	108.95	0.59	0.59	0.59	-0.54	-0.54	-0.54
0.90	11.89	11.91	11.85	117.22	117.79	116.07	0.79	0.87	0.62	-0.48	-0.43	-0.58
0.80	26.41	26.54	26.03	129.91	132.31	124.80	0.95	1.10	0.64	-0.43	-0.33	-0.65
0.70	44.97	45.43	43.41	148.90	154.70	135.72	1.08	1.26	0.66	-0.38	-0.23	-0.76
0.60	70.02	71.14	65.39	177.47	188.82	149.83	1.19	1.38	0.68	-0.32	-0.12	-0.95
0.50	106.24	108.58	94.40	221.94	242.16	168.79	1.26	1.45	0.70	-0.27	-0.02	-1.41
0.40	163.56	168.11	134.99	295.77	330.74	195.77	1.31	1.50	0.72	-0.21	0.09	-3.97
0.30	267.06	275.94	197.14	432.89	495.07	237.71	1.34	1.52	0.74	-0.16	0.19	2.65
0.20	500.24	519.34	308.15	745.97	869.91	313.53	1.35	1.52	0.75	-0.11	0.29	0.77

The variation of Barton-Stacey Gruneisen Parameter $\gamma_{ba\text{-}s}$ versus V/V_0 by using Brennan-Stacey EOS, Shanker EOS and Vinet EOS for transition metals [Fig. (1-10)]

Fig. 1

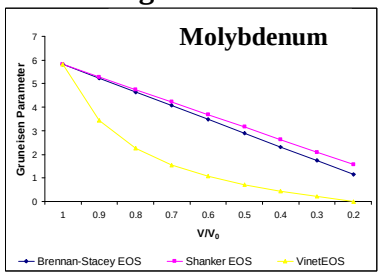


Fig. 2

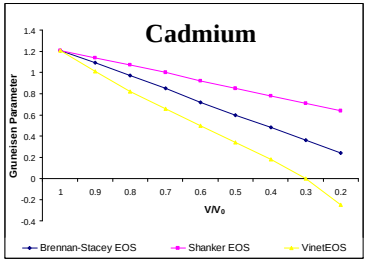


Fig. 3

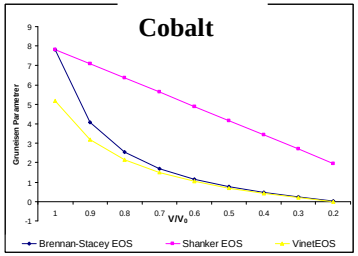


Fig. 4

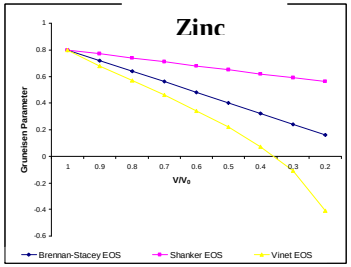


Fig. 5

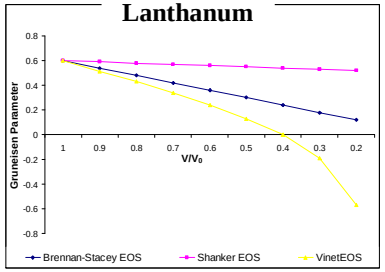


Fig. 6

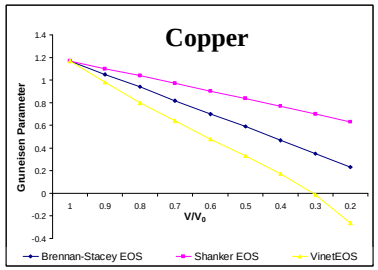


Fig. 7

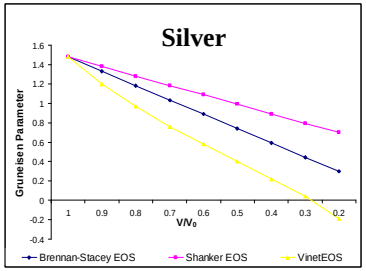


Fig. 8

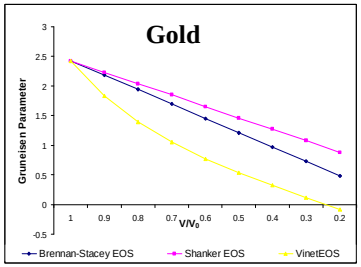


Fig. 9

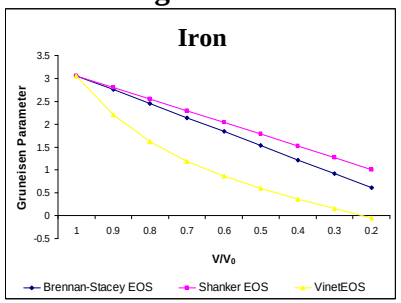
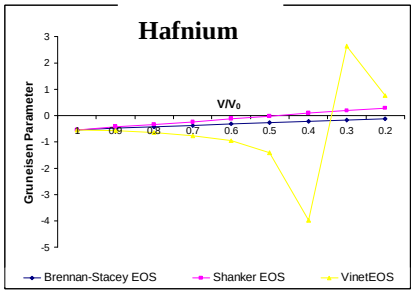


Fig. 10



calculated by using Shanker EOS is the best equation of state for calculating Grüneisen parameter both at high and low compression ranges for elements.

The calculated values of pressure (P), isothermal bulk modulus (K_T), its first pressure derivative ($\mathbf{K}_T'$), Barton-Stacey Grüneisen parameter ($\gamma_{ba\text{-}s}$) and Anderson-Grüneisen parameter (δ_T) at different compressions (V/V_0) for ten transition metals; Mo, Cd, Co, Zn, La, Cu, Ag, Au, Fe and Hf; at $T=T_0=300K$, are given in the tables- (2 -11) respectively.

The graph showing the variation of Barton-Stacey Gruneisen Parameter $\gamma_{ba\text{-}s}$ versus V/V_0 by using Brennan-Stacey EOS, Shanker EOS and Vinet EOS for ten transition metals; Mo, Cd, Co, Zn, La, Cu, Ag, Au, Fe and Hf; are shown in Fig.(1 – 10) respectively. These graphs are in good agreement with the above explanation.

Also the Anderson-Grüneisen parameter calculated by using equation (13), shows that Anderson-Grüneisen (δ_T) decreases with increasing pressure. For the change in volume under the effect of pressure following form have been pointed out for Anderson-Grüneisen (δ_T) [25]

$$\frac{\delta_T + 1}{V / V_0} = A \qquad \text{and} \qquad \delta_T = \delta_{T_0}\left(\frac{V}{V_0}\right)^k$$

where A and k are constants. These equations are most consistent in high pressure research.

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