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Gruneisen parameter for bulk metallic glasses under extreme compression

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ABSTRACT

The Grüneisen parameter (γ) is of considerable importance to Earth scientists because it sets limitations on the thermoelastic properties of the lower mantle and core. The Grüneisen parameter is directly related to the equation of state (EOS), yet it is often the case that both the form of □□and the EOS are chosen independently of each other and somewhat arbitrarily. In this paper the volume dependence of Gruneisen parameter has been calculated by using three different phenomenological isothermal EOS viz. Brennan Stacey EOS, Shanker EOS and Vinet EOS for five different bulk metallic glasses viz. $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$, $Zr_{41}Ti_{14}Cu_{12.5}Ni_{9}Be_{22.5}C_{1}$, $Zr_{40}Nb_{8}Cu_{12}Fe_{8}Be_{24}$, $(Zr_{0.59}Ti_{0.06}Cu_{0.22}Ni_{0.13})_{85.7}Al_{14.3}$ and $Pd_{39}Ni_{10}Cu_{30}P_{21}$. For calculation of Gruneisen parameter we have consider Barton – Stacey relation.On analysis of of result thus obtained shows that Shanker EOS is best EOS for calculating Gruneisen parameter both under high as well as low compression ranges.

Introduction

The Grüneisen parameter is an important quantity for studying the thermoelastic behavior of bulk metallic glasses at high pressures and temperatures. Bulk metallic glasses (BMGs) exhibit many attractive properties such as high strength, high-specific strength, excellent corrosion and wear resistance, and near-net-shape processibility. From the structural perspective, the thermo elastic behavior BMGs correlates with their atomic scale structure, asymmetry of short-range ordered clusters and their fraction[1]. However, characterization and visualization of metallic glass structure remains a challenging and tedious task even for computer simulation. The study of the pressure (volume) dependence of γ is an interesting problem from theoretical as well as experimental point of view, particularly, due to the lack of a proper theory and enough experimental data [2].

The value for γ is used to place constraints on geophysically important parameters such as the pressure and temperature dependence of the thermal properties of the mantle and core, the adiabatic temperature gradient and the geophysical interpretation of Hugoniot data[3]. It is an approximately constant, dimensionless parameter that varies slowly as a function of pressure and temperature. The Gruneisen parameter 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 thermodynamic properties such as heat capacity and thermal expansion. Unfortunately, the experimental determination of γ, defined in either way, is extremely difficult; the microscopic definition requires a detailed knowledge of the phonon dispersion spectrum of a material, whereas the macroscopic definition requires experimental measurements of thermodynamic properties at high pressures and temperatures. As a result of the difficulty associated with obtaining experimentally an accurate value for γ, a number of more approximate expressions have been suggested [4]. Many of these expressions relate γ at atmospheric pressure (P = 0) to the first derivative of the bulk modulus with respect to pressure (K'_T), via $\gamma = 1/2K'_T - x$, where x is a constant. These relations may be expanded to take into account the variation of γ with pressure. In these more general cases, γ (P) is a function of the equation of state. Despite the intrinsic relationship between γ and the EOS [5], 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 values of γ for many geologically relevant materials.

In present work the volume dependence of Gruneisen parameter has been calculated by using three different phenomenological isothermal EOS viz. Brennan Stacey EOS, Shanker EOS and Vinet EOS for five different bulk metallic glasses viz. $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$, $Zr_{41}Ti_{14}Cu_{12.5}Ni_{9}Be_{22.5}C_{1}$, $Zr_{48}Nb_{8}Cu_{12}Fe_{8}Be_{24}$, $(Zr_{0.59}Ti_{0.06}Cu_{0.22}Ni_{0.13})_{85.7}Al_{14.3}$ and $Pd_{39}Ni_{10}Cu_{30}P_{21}$.

Theory:

Equation of states are derived on taking account of some basic assumptions. Brennan-Stacey EOS[6,7] is based on assumption that Gruniesen parameter is proportional to volume and equation is obtained on account of free volume formula[8],given as follows

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

On the basis of a modified exponential dependence for the short range force constant on volume, the Shanker EOS[9,10] is derived, given as follows:

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

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Where, $y = 1 - \frac{V}{V_0}$ and $t = K_0^{'} - \frac{8}{3}$

Taking account universal relationship between binding energy and interatomic separation for solids, Vinet EOS [11,12,13] derived given as follows:

$$P = 3K_0 x^{-2}(1-x)\exp\{\eta(1-x)\} \tag{3}$$

Where, $x = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and $\eta = \frac{3}{2}\left(K_0^{'} - 1\right)$

Isothermal Bulk modulus K_T can be obtained by taking first volume derivative of above three relations as follows:

$$K_T = -V\left(\frac{\partial P}{\partial V}\right)_T \tag{4}$$

Thus taking differentiation of above three pressure-volume relations with respect to volume and putting in equation (4), expressions for isothermal bulk modulus is derived as follows:

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

$$K_T = \frac{4}{3}P + K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}\exp\left\{\left(K_0^{'} - \frac{8}{3}\right)\left(1 - \frac{V}{V_0}\right)\right\} \tag{6}$$

$$K_T = K_0 x^{-2}\left[1 + \{(1+\eta x)(1-x)\}\right]\exp \eta(1-x) \tag{7}$$

Pressure derivative of isothermal bulk modulus K_T gives first pressure derivative of bulk modulus $K_T^{'}$ as follows:

$$K_T^{'} = \frac{16}{9}\frac{P}{K_T} + \left(1 - \frac{4}{3}\frac{P}{K_T}\right)\left[\left\{\left(K_0^{'} - \frac{5}{3}\right)\left(\frac{V}{V_0}\right)\right\} + \frac{5}{3}\right] \tag{8}$$

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

$$K_T^{'} = \frac{1}{3}\left[\frac{x(1-\eta) + 2\eta x^2}{1 + (\eta x + 1)(1-x)} + \eta x + 2\right] \tag{10}$$

Now from derivative of above expressions (equations 8-10) w.r.t. P, second order pressure derivative of bulk modulus in terms of $K_T K_T^{''}$ is obtained as follows:

$$K_T K_T^{''} = \frac{4}{3}\left(1 - \frac{PK_T^{'}}{K_T}\right)\left[\frac{4}{3} - \left\{\frac{V}{V_0}\left(K_0^{'} - \frac{5}{3}\right) + \frac{5}{3}\right\}\right] - \left(\frac{V}{V_0}\right)\left(K_0^{'} - \frac{5}{3}\right)\left(1 - \frac{4}{3}\frac{P}{K_T}\right) \tag{11}$$

$$K_T K_T^{''} = \frac{4}{3}\left(1 - \frac{PK_T^{'}}{K_T}\right)\left[\frac{4}{3} - \left\{\frac{V}{V_0}\left(K_0^{'} - \frac{8}{3}\right) + \frac{8}{3}\right\}\right] - \left(\frac{V}{V_0}\right)\left(K_0^{'} - \frac{8}{3}\right)\left(1 - \frac{4}{3}\frac{P}{K_T}\right) \tag{12}$$

$$K_T K_T^{''} = -\frac{x}{9}\left[\frac{\{(1-\eta) + 4\eta x\} - \{(3K_T^{'} - \eta x - 2)(\eta - 2\eta x - 2)\}}{\{1 + (\eta x + 1)(1-x)\}} + \eta\right] \tag{13}$$

Equations (1), (5), (8) and (11) corresponds to Brennan-Stacey EOS. Equation (2) , (6), (9) and (12) corresponds to Shanker EOS. Equations (3),(7),(10)and (13)corresponds to Vinet EOS. In the above equations K_0 is isothermal bulk modulus and $K_0^{'}$ is the first pressure derivative of isothermal bulk modulus at zero pressure value.

Gruniesen parameter γ derived by Barton-Stacey [14,15] is given by following expression:

$$\gamma = \frac{\frac{1}{2}K_T^{'} - \frac{1}{6} - \frac{f}{3}\left(1 - \frac{P}{3K_T}\right)}{\left(1 - \frac{4}{3}\frac{P}{K_T}\right)}$$

Result and Discussion

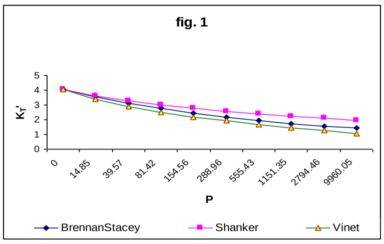
In the present work we have calculated pressure P, corresponding to different compression ranges $\frac{V}{V_0}$ =1.00 to V/V_0 = 0.1for five bulk metallic glasses viz. $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$, $Zr_{41}Ti_{14}Cu_{12.5}Ni_9Be_{22.5}C_1$, $Zr_{40}Nb_8Cu_{12}Fe_8Be_{24}$, $(Zr_{0.59}Ti_{0.06}Cu_{0.22}Ni_{0.13})_{85.7}Al_{14}$ and $Pd_{39}Ni_{10}Cu_{30}P_{21}$ by using three different empirical isothermal equations of state viz. Brennan-Stacey EOS, Shanker EOS and Vinet EOS given by equation. Equation (1) corresponds to Brennan and Stacey EOS, equation (2) corresponds to Shanker EOS and equation (3) corresponds to Vinet EOS. All three EOS's need two input parameters, the input values of K_0 and $K_0^{'}$ displayed in table-1, taken from literature [15, 16]. The value of pressure P as calculated by using equations (1-3) putting in the equations (5-7), we obtain the value of isothermal bulk modulus K_T as displayed in table (2-6). Further substituting the value of K_T as calculated by using equation (5-7) in equation (8-10) the value of first pressure derivative of isothermal bulk modulus $K_T^{'}$ has been obtained corresponding to different compressions displayed in table (2-6).

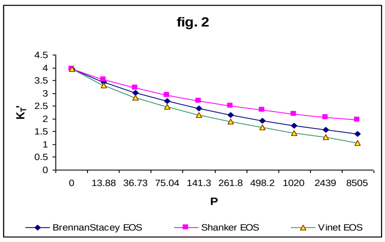
Again after substituting the values of P, K_T and $K_T^{'}$ calculated as above in equation (11-13), $K_T K_T^{''}$ has been calculated displayed in table (2-6).

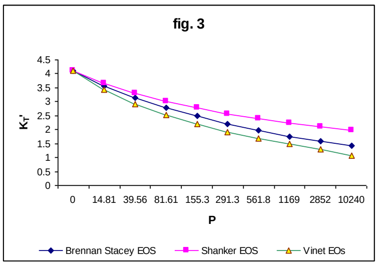
Further substituting the values of P, K_T and $K_T^{'}$ calculated by using equation (1-10) in equation (14) the value of Gruneisen parameter has been obtained at different compressions displayed in table (2-6).

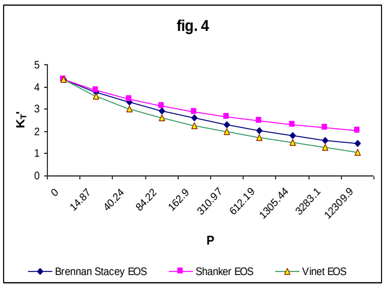
The graphs plotted between P vs $K_T^{'}$ displayed in fig. (1-5), P vs $K_T K_T^{''}$ displayed in fig.(6-10) and $\frac{V}{V_0}$ vs γ displayed in fig.(11-15). After making the analysis of the graphs, it is observed that from fig. (1-5), $K_T^{'}$ decreases as the pressure P gets increased.

It verify the constraint which states that the pressure derivative of isothermal bulk modulus must decreases progressively with the increase in pressure [17, 18]. Again when analyzing the EOS critically Stacey given a constraint states that At extreme compression $P \to \infty$ and $\frac{V}{V_0} \to 0$, $K_\infty^{'}$ must be greater than $\frac{5}{3}$.









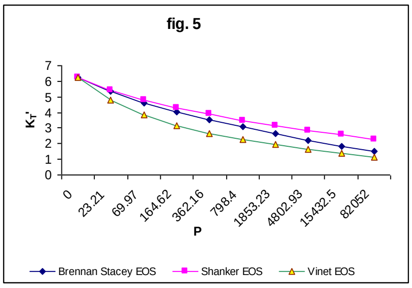
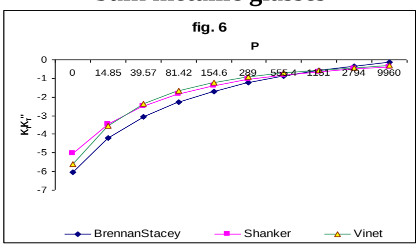
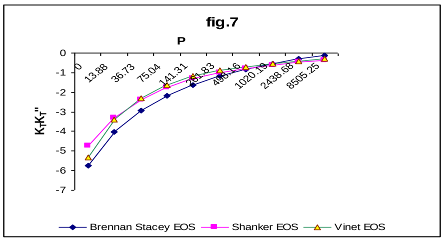
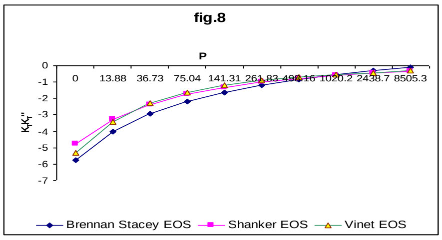
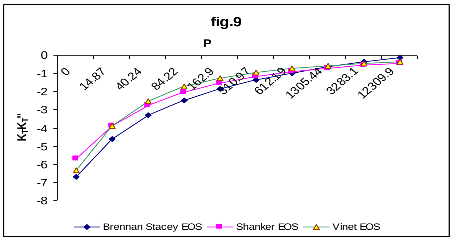


Figure (1-5): The variation of pressure P versus K_T' by using Brennan-Stacey EOS, Shanker EOS and Vinet EOS for bulk metallic glasses









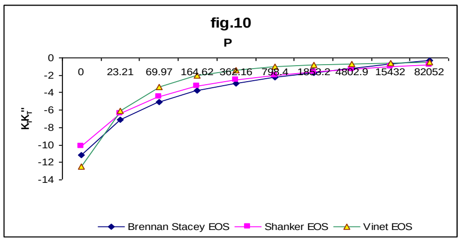


Figure (6-10): The variation of pressure P versus $K_T K_T''$ by using Brennan-Stacey EOS, Shanker EOS and Vinet EOS for bulk metallic glasses

When we analyzing extreme compression behavior of BMG's (we have taken $\frac{V}{V_0} = 1\times10^{-7}$) we found that at extreme compression when the value of K_T' i.e. K_∞' is calculated by using Brennan-Stacey EOS it comes to $K_\infty' \approx \frac{4}{3}$, which shows that K_∞' is characteristic of EOS and not of the metal. Whereas in case of Shanker EOS, K_∞' is found to varying from 1.87 to 2.05 i.e. $K_\infty' \geq \frac{5}{3}$ which shows that K_∞' is characteristic of the metal and not the EOS. Again when we calculated K_∞' by using Vinet EOS, it is found that $K_\infty' \approx 0.67$ i.e. $K_\infty' \approx \frac{2}{3}$ for all the bulk metallic glasses, which shows that K_∞' is characteristic of EOS and not of the metal. Stacey [17, 18] has made a constraint regarding K_∞' states that $K_\infty' \geq \frac{5}{3}$ and is characteristic of metal which strongly supports the Shanker EOS for calculating Gruneisen parameter at different compression ranges. The above work has also been verified by Holzapfel [19, 20].

The real test of an EOS can be presented by using a well accepted constraint. According to first constraint $K_0 K_0''$ must be negative which support strongly the work of literature [21] and have no contradiction. From fig. (6-10), it is clear that the graph plotted between P vs $K_T K_T''$ remains always negative which strongly supports the above constraint. It depends upon the fact that K_T' decreases with the increase in pressure. This is supported theoretically, as well as experimentally [18].

Further for P →0, i.e. $\frac{V}{V_0} \rightarrow 1$ equation (11-13) reduces to

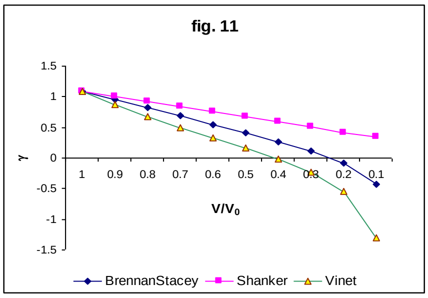
$$K_0K_0'' = \frac{31}{4} - \frac{7}{3}K_0' \qquad (15)$$

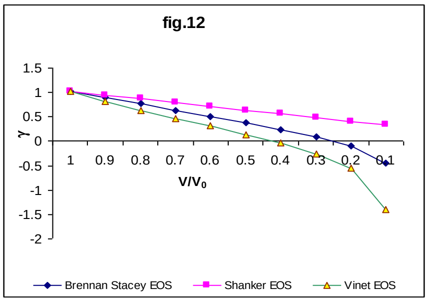
$$K_0K_0'' = \frac{40}{9} - \frac{7}{3}K_0' \qquad (16)$$

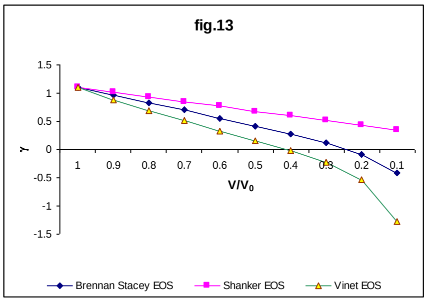
$$K_0K_0'' = \frac{19}{36} - \frac{K_0'}{2} - \frac{K_0'^2}{4} \qquad (17)$$

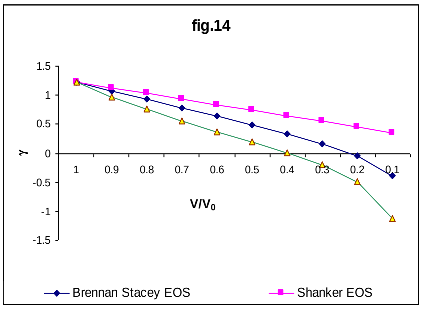
When we substitute the values of K_0' from table (1) in equations (15 – 17) it is found that each EOS's as discussed above provides a negative value of K_0K_0''. It also conclude that there is no contradiction regarding evaluation of K_0K_0'' by using different EOS for BMG's.

Again when we analyzing the graph plotted between γ vs V/V_0 by using different isothermal EOS as shown in fig. (11 – 15), it is found that the nature of graph is always straight line in case of Shanker EOS where as it is curved in case of Brennan-Stacey EOS and Vinet EOS at higher compression. For better approximation Fang and Rong [22] and also A. K. Pandey etal [23] has suggested that γ vs V/V_0 curve must be straight line which strongly supports the Shanker EOS for calculating Gruneisen parameter both at high as well as low pressure ranges whereas Vinet EOS and Brennan – Stacey EOS is applicable only at low compression ranges for calculating Gruneisen parameter at different compressions.









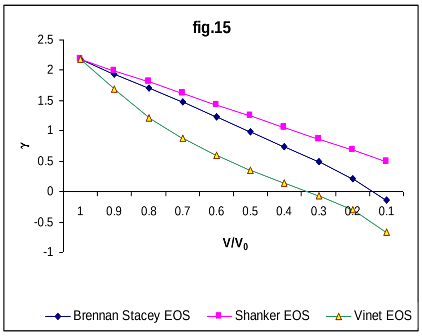


Figure (11-15): The variation of γ versus V/V_0 by using Brennan-Stacey EOS, Shanker EOS and Vinet EOS for bulk metallic glasses

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Table1: Input value of Bulk modulus (K_0) and its first pressure derivative ($K_0^{'}$) for different bulk metallic glasses at zero pressure [10, 11]

S.No	Element	K_0 (GPa)	$K_0^{'}$
1	$Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$	78.89	3.17
2	$Zr_{41}Ti_{14}Cu_{12.5}Ni_9Be_{22.5}C_1$	40.43	4.28
3	$Zr_{48}Nb_8Cu_{12}Fe_8Be_{24}$	2.86	7.20
4	$(Zr_{0.59}Ti_{0.06}Cu_{0.22}Ni_{0.13})_{85.7}Al_{14.3}$	9.46	1.73
5	$Pd_{39}Ni_{10}Cu_{30}P_{21}$	30.97	4.09

Table2: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative ($K_T^{'}$), $K_T K_T^{''}$ and Barton-Stacey Grüneisen parameter (γ) at different compressions (V/V_0) for $Zr_{41}Ti_{14}Cu_{12.5}Ni_{10}Be_{22.5}$ 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)	K_T'(b)	K_T '(c)	K_TK_T"(a)	K_TK_T"(b)	K_TK_T"(c)	γ (a)	γ (b)	γ (c)
1	0	0.00	0	114.1	114.1	114.1	4.06	4.06	4.06	-6.03	-5.03	-5.62	1.08	1.08	1.08
0.9	14.84	14.86	14.85	169.91	170.75	170.29	3.53	3.62	3.39	-4.2	-3.47	-3.55	0.95	1	0.87
0.8	39.41	39.65	39.57	250.91	255.88	253.37	3.11	3.28	2.89	-3.05	-2.49	-2.37	0.82	0.92	0.68
0.7	80.56	81.61	81.42	370.9	387.65	379.85	2.76	2.99	2.5	-2.26	-1.84	-1.66	0.69	0.84	0.5
0.6	151.18	154.44	154.56	553.94	599.59	580.05	2.46	2.76	2.18	-1.69	-1.39	-1.21	0.55	0.76	0.33
0.5	277.39	286.12	288.96	845.56	958.55	914.1	2.19	2.56	1.92	-1.24	-1.06	-0.92	0.41	0.67	0.16
0.4	518.25	539.99	555.43	1342	1613.17	1514.74	1.96	2.38	1.68	-0.88	-0.82	-0.71	0.27	0.59	-0.02
0.3	1030.4	1084.43	1151.35	2284.11	2952.66	2724.03	1.75	2.23	1.47	-0.58	-0.64	-0.56	0.11	0.51	-0.23
0.2	2357.9	2505.06	2794.46	4467.59	6314.07	5675.31	1.57	2.09	1.28	-0.33	-0.5	-0.44	-0.09	0.42	-0.54
0.1	7825.8	8384.14	9960.05	12553.2	19793.2	16589.17	1.43	1.97	1.07	-0.12	-0.38	-0.32	-0.43	0.34	-1.3

Table3: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative ($K_T^{'}$), $K_T K_T^{''}$ and Barton-Stacey Grüneisen parameter (γ) at different compressions (V/V_0) for $Zr_{41}Ti_{14}Cu_{12.5}Ni_9Be_{22.5}C_1$ 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)	K_T'(b)	K_T '(c)	K_TK_T"(a)	K_TK_T"(b)	K_TK_T"(c)	γ (a)	γ (b)	γ (c)
1	0	0	0	107.3	107.3	107.3	3.94	3.94	3.94	-5.75	-4.75	-5.32	1.02	1.02	1.02
0.9	13.86	13.89	13.88	157.99	158.77	158.35	3.43	3.52	3.31	-4.02	-3.3	-3.41	0.89	0.94	0.82
0.8	36.59	36.81	36.73	230.9	235.46	233.17	3.03	3.2	2.83	-2.93	-2.38	-2.3	0.77	0.87	0.64
0.7	74.26	75.21	75.04	338.02	353.23	346.08	2.69	2.93	2.46	-2.17	-1.76	-1.62	0.64	0.79	0.47
0.6	138.29	141.24	141.31	500.22	541.18	523.17	2.41	2.7	2.15	-1.62	-1.32	-1.19	0.51	0.72	0.31
0.5	251.71	259.55	261.83	756.91	857.13	815.82	2.15	2.51	1.89	-1.19	-1.01	-0.9	0.38	0.64	0.14
0.4	466.32	485.66	498.16	1191.43	1429.16	1336.53	1.93	2.34	1.67	-0.84	-0.78	-0.7	0.24	0.57	-0.04
0.3	919	966.64	1020.19	2012.38	2591.64	2372.73	1.73	2.2	1.46	-0.55	-0.61	-0.55	0.09	0.49	-0.25
0.2	2083.8	2212.31	2438.68	3909.28	5490.49	4867.19	1.56	2.07	1.27	-0.31	-0.47	-0.43	-0.1	0.41	-0.56
0.1	6850.6	7333.63	8505.25	10922.7	17049.9	13929.24	1.43	1.96	1.06	-0.12	-0.36	-0.31	-0.45	0.33	-1.4

Table 4: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), $K_T K_T''$ and Barton-Stacey Grüneisen parameter (γ) at different compressions (V/V_0) for $Zr_{48}Nb_8Cu_{12}Fe_8Be_{24}$ 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)	K_T'(b)	K_T'(c)	K_TK_T''(a)	K_TK_T''(b)	K_TK_T''(c)	γ (a)	γ (b)	γ (c)
1	0	0	0	113.6	113.6	113.6	4.1	4.1	4.1	-6.12	-5.12	-5.72	1.1	1.1	1.1
0.9	14.8	14.82	14.81	169.81	170.65	170.19	3.56	3.65	3.42	-4.25	-3.53	-3.6	0.97	1.02	0.88
0.8	39.41	39.65	39.56	251.63	256.61	254.08	3.14	3.3	2.91	-3.09	-2.53	-2.4	0.83	0.93	0.69
0.7	80.75	81.8	81.61	373.16	390.04	382.19	2.78	3.02	2.51	-2.29	-1.87	-1.67	0.7	0.85	0.51
0.6	151.92	155.21	155.34	559.04	605.21	585.58	2.48	2.78	2.19	-1.71	-1.41	-1.22	0.56	0.77	0.33
0.5	279.5	288.32	291.27	855.85	970.56	926.06	2.21	2.57	1.92	-1.26	-1.08	-0.92	0.42	0.68	0.16
0.4	523.67	545.72	561.8	1362.12	1638.5	1540.38	1.97	2.39	1.69	-0.9	-0.83	-0.72	0.28	0.6	-0.02
0.3	1044.3	1099.25	1169.27	2324.36	3008.4	2782.07	1.76	2.24	1.48	-0.59	-0.65	-0.57	0.12	0.52	-0.23
0.2	2397	2547.23	2852.4	4556.83	6453.54	5826.34	1.58	2.1	1.28	-0.33	-0.5	-0.45	-0.08	0.43	-0.53
0.1	7981.2	8552.83	10240.4	12828.5	20294.8	17151.18	1.43	1.98	1.07	-0.13	-0.39	-0.32	-0.42	0.34	-1.27

Table 5: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T'), $K_T K_T''$ and Barton-Stacey Grüneisen parameter (γ) at different compressions (V/V_0) for $(Zr_{0.59}Ti_{0.06}Cu_{0.22}Ni_{0.13})_{85.7}Al_{14.3}$ 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)	K_T'(b)	K_T'(c)	K_TK_T''(a)	K_TK_T''(b)	K_TK_T''(c)	γ (a)	γ (b)	γ (c)
1	0	0	0	112.6	112.6	112.6	4.34	4.34	4.34	-6.68	-5.68	-6.35	1.22	1.22	1.22
0.9	14.86	14.88	14.87	172.18	173.03	172.52	3.76	3.85	3.58	-4.6	-3.87	-3.88	1.07	1.13	0.97
0.8	40.09	40.34	40.24	260.49	265.67	262.91	3.3	3.46	3.02	-3.32	-2.76	-2.53	0.93	1.03	0.76
0.7	83.25	84.45	84.22	393.94	411.89	403.4	2.92	3.15	2.6	-2.47	-2.03	-1.74	0.78	0.94	0.56
0.6	159.26	162.77	162.9	601.29	651.56	630.57	2.59	2.89	2.25	-1.85	-1.53	-1.26	0.64	0.84	0.37
0.5	297.85	307.44	310.97	973.13	1064.97	1018.29	2.3	2.67	1.97	-1.37	-1.18	-0.95	0.49	0.75	0.19
0.4	567.78	592.2	612.19	1517	1832.3	1732.69	2.04	2.47	1.72	-0.98	-0.92	-0.74	0.33	0.65	0.01
0.3	1152.9	1214.95	1305.44	2629.96	3428.83	3210.94	1.81	2.3	1.5	-0.65	-0.72	-0.59	0.16	0.56	-0.2
0.2	2696.6	2869.47	3283.1	5229.81	7497.71	6936.49	1.6	2.15	1.3	-0.37	-0.56	-0.47	-0.04	0.46	-0.48
0.1	9155.6	9826.1	12309.9	14897.7	24039	21302.9	1.44	2.02	1.08	-0.14	-0.43	-0.34	-0.38	0.36	-1.13

Table6: Calculated values of pressure (P) , isothermal bulk modulus (K_T), its first pressure derivative (K_T') and Barton-Stacey Grüneisen parameter (γ_{ba-s}) at different compressions (V/V_0) for $Pd_{39}Ni_{10}Cu_{30}P_{21}$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)	K_T'(b)	K_T'(c)	K_TK_T''(a)	K_TK_T''(b)	K_TK_T''(c)	γ (a)	γ (b)
0	0	0	159.1	159.1	159.1	6.27	6.27	6.27	-11.19	-10.19	-12.44	2.19	2.19	2.19
23.25	23.29	23.21	292.12	293.58	291	5.33	5.43	4.77	-7.14	-6.38	-6.04	1.94	1.99	1.69
70.32	70.79	69.97	524.1	534.8	519.84	4.63	4.81	3.82	-5.05	-4.42	-3.33	1.71	1.81	1.21
165.65	168.07	164.62	933.82	978.63	929.55	4.05	4.31	3.15	-3.8	-3.28	-2.04	1.477	1.62	0.88
362.31	371.37	362.16	1672.4	1823.87	1696.65	3.53	3.88	2.65	-2.93	-2.55	-1.39	1.23	1.43	0.6
783.02	811.98	798.4	3046.71	3512.03	3225.96	3.07	3.5	2.26	-2.26	-2.04	-1.04	0.99	1.25	0.36
1739.3	1825.72	1853.23	5737.56	7124.6	6562.88	2.63	3.16	1.94	-1.69	-1.65	-0.85	0.74	1.06	0.15
4145.2	4403.09	4802.93	11489.1	15739.9	14916.24	2.22	2.85	1.66	-1.17	-1.33	-0.73	0.49	0.87	-0.07
11451	12295.2	15432.5	26083.3	40690.8	41314.6	1.85	2.56	1.4	-0.69	-1.05	-0.63	0.22	0.68	-0.3
46160	50009.5	82052	83138	154464	178747.6	1.54	2.3	1.15	-0.27	-0.78	-0.51	-0.14	0.5	-0.66