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Equations of state for metals under high compression

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Abstract

The extreme compression value of the pressure derivative of bulk modulus *i.e.* K_∞' has been treated as an adjustable parameter in recent studies on high pressure equations of state (EOS) for solids. The present study presents the elastic behaviour of metals *i.e.* Iron, Aluminium and Copper under high compression with the help of Birch-Murnaghan, Bre-Stacey, Shanker, Born, Vinet, Bardeen, Ullaman and Tait Equations of state.

Further these EOS have been critically examined by evaluating the values of pressure derivative of bulk modulus at infinite pressure. The value of this parameter is found out to be grater than 5/3 by some EOS in case of Fe, Al and Cu such results is in good agreement with the Seismic Study of these metals.

Key words: Elastic Behaviour, High Compression, Equation of state.

Introduction

The equation of state (EOS) of a solid describes the relationship among thermodynamic variables such as pressure, temperature, and volume. It provides numerous information of non-linear compression of a material at high pressure and has been widely applied to engineering and other scientific researcher. Recently, rapid advances in computational techniques have extremely promoted the theoretical works. Significant progress has been achieved over the past year to describe the properties of condensed matter in terms of universal relationship involving a small number of parameters. Especially since 1984 Rose *et al.*[1] proposed that there exists a universal EOS (UEOS) K_∞' forms of UEOS have been proposed with different extent of success[2-20].

The extreme compression $(V \rightarrow 0)$ value of the pressure derivative of bulk modulus *i.e.* K_∞' has been treated as an adjustable parameter in recent studies on high- pressure equation of state (EOS) for solids [20-22].

It has been emphasized that $K_\infty{}'$ is an important EOS parameter. A careful inspection of Table 1 given by Stacey[23] reveals that there are two types of EOS. In first category are those equation with yield a fixed numerical value of $K_\infty{}'$. Thus value of is a characteristic property[24] of the EOS and it is same for all types of material to which the EOS is applied. The value of is $K_\infty{}'$ is changed only when one EOS is replaced by the other. Several EOS [23-26] have been formulated such that $K_\infty{}'$=5/3. There has been a long list of workers [24-27] and references given therein who have provided a fundamental support to this value (5/3) of $K_\infty{}'$ on the basis of the Thomas-Fermi model applicable at extreme compression.

Stacey [23,29] does not agree with the Thomas-Fermi model. He believes that solids even at extreme compression do not resemble with the Thomas-Fermi electron gas, therefore $K_\infty{}'$=5/3 should be rejected. Stacey[29] developed a new constraints $K_\infty{}'$>5/3 on the basis of thermodynamics in the limit of infinite pressure. But this is also subject to the criticism recently made by Shanker et al.[32] on the basis of the generalized theory of the Grüneisen parameter [31].

The second type of EOS includes those equations which treat $K_\infty{}'$ as an adjustable parameter. For such equations $K_\infty{}'$ is not a characteristic parameter of the EOS, but is depends on the material to which the EOS is applied. Thus $K_\infty{}'$ is a property of the given solid in the same sense as the zero pressure parameters K_T and $K_T{}'$ representing bulk modulus and its pressure derivative. The most striking point is that $K_\infty{}'$ which is an infinite pressure parameter is directly related to the zero-pressure parameter. The role of $K_\infty{}'$ in different equations of state is investigated in the present paper.

Theory :

An EOS for metals provide useful information between Pressure(P), Bulk modulus (K_T) and Pressure derivative of bulk modulus (K'_T) which help us to understand the behaviour of the material under the effect of high pressure and high temperature.In the following we write out Birch-Murnaghan(B-M), Bre-Stacey (B-S), Born (Bo), Shanker (Sh), Hama-suito(H-S) Vinet(Vin), Bardeen (Bar), Ullmann (Ull), Tait(T) and Slater(Sl) EOS for later convenience.

Pressure P For Metals (Fe, Al And Cu):

$$P_{Birch-Mur.} = \frac{3}{2} K_0(x^{-7} - x^{-5}) \left[1 + \frac{3}{4}(K_0{}' - 4)(x^{-2} - 1)\right] \qquad \text{---- } 1a$$

$$P_{Bren.-Stacey} = \frac{3K_0(V/V_0)^{-4/3}}{(3K_0{}'-5)} \left[\left\{exp\frac{(3K_0{}'-5)}{3} \times \left(1 - \frac{V}{V_0}\right)\right\} - 1\right] \qquad \text{---- } 1b$$

$$P_{Shanker} = \frac{K_0(V/V_0)^{-4/3}}{t} \left[\left(1 - \frac{1}{t} + \frac{2}{t^2}\right)\{exp(ty) - 1\} + y\left(1 + y - \frac{1}{t}\right)exp(ty)\right] \qquad \text{---- } 1c$$

$$P_{Born} = \frac{3K_0}{(3K_0{}' - 8)} \left[\left(\frac{V}{V_0}\right)^{4/3-K_0{}'} - \left(\frac{V}{V_0}\right)^{-4/3}\right] \qquad \text{---- } 1d$$

$$P_{Vinet} = 3K_0\left[\frac{1-x}{x^2}\right]e^{\eta[1-x]} \qquad \text{---- } 1e$$

$$P_{Hama-suito} = 3K_0 x^{-5}(1 - x)exp\left[(\eta - 3)(1 - x) + \left(\xi - \frac{3}{2}\right)(1 - x)^2\right] \qquad \text{---- } 1f$$

$$P_{Bardeen} = 3K_0 \left[\left(\frac{V}{V_0} \right)^{-5/3} - \left(\frac{V}{V_0} \right)^{-4/3} \right] \left\{ 1 + \frac{3}{2} (K_0' - 3) \left[\left(\frac{V}{V_0} \right)^{-1/3} - 1 \right] \right\} \qquad \text{---- } 1g$$

$$P_{Ullmann} = \frac{3K_0}{(K_0'-2)} \left[\left(\frac{V}{V_0} \right)^{-\left(\frac{2K_0'-1}{3} \right)} - \left(\frac{V}{V_0} \right)^{-\left(\frac{(K_0'+1)}{3} \right)} \right] \qquad \text{---- } 1h$$

$$P_{Tait} = \frac{K_0}{(K_0'+1)} \left[exp \left\{ (K_0' + 1) \left(1 - \frac{V}{V_0} \right) \right\} - 1 \right] \qquad \text{---- } 1i$$

$$P_{Slater} = K_0 \left(1 - \frac{V}{V_0} \right) + \frac{1}{2} K_0 (K_0' + 1) \left(1 - \frac{V}{V_0} \right)^2 \text{------} 1j$$

Relationship :

$$a = \frac{3}{2} (K_0' - 4) , \quad t = K_0' - \frac{8}{3} , \quad y = 1 - \frac{V}{V_0} , \quad \eta = \frac{3}{2} (K_0' - 1), \quad x = \left(\frac{V}{V_0} \right)^{1/3}$$

On the basis of above relations for Pressure (P) and other parameters. The relations for the bulk modulus and its pressure derivative have been derived. These relations are given below.

Bulk Modulus K_T For Metals (Fe, Al And Cu):

$$K_{T\,Birch-Mur.} = \frac{1}{2} K_0 (7x^{-7} - 5x^{-5}) + \frac{3}{8} K_0 (K_0' - 4)(9x^{-9} - 14x^{-7} + 5x^{-5}) \qquad \text{---- } 2a$$

$$K_{T\,Bren.-Stacey} = K_0 \left(\frac{V}{V_0} \right)^{-1/3} exp \left\{ \left(K_0' - \frac{5}{3} \right) \left(1 - \frac{V}{V_0} \right) \right\} + \frac{4}{3} P \qquad \text{---- } 2b$$

$$K_{T\,Shanker} = K_0 \left(\frac{V}{V_0} \right)^{-4/3} exp \left\{ \left(K_0' - \frac{8}{3} \right) \left(1 - \frac{V}{V_0} \right) \right\} + \frac{4}{3} P \qquad \text{---- } 2c$$

$$K_{T\,Born} = K_0 \left(\frac{V}{V_0} \right)^{\frac{4}{3} - K_0'} + \frac{4}{3} P \qquad \text{---- } 2d$$

$$K_{T\,Vinet} = K_0 \left[\frac{\eta(1-x)}{x} + \frac{(2-x)}{x^2} \right] e^{\eta[1-x]} \qquad \text{---- } 2e$$

$$K_{T\,Hama-suito} = \frac{P}{3} \left[5 + \frac{x}{(1-x)} + x\{\eta + 2\xi(1-x) + 3x - 6\} \right] \qquad \text{---- } 2f$$

$$K_{T\,Bardeen} = K_0 \left[2(3K_0' - 11) \left(\frac{V}{V_0} \right)^{-4/3} - 5(3K_0' - 10) \left(\frac{V}{V_0} \right)^{-5/3} + 3(3K_0' - 9) \left(\frac{V}{V_0} \right)^{-2} \right] \qquad \text{---- } 2g$$

$$K_{T\,Ullmann} = \frac{K_0}{(K_0'-2)} \left[(2K_0' - 1) \left(\frac{V}{V_0} \right)^{-\left(\frac{2K_0'-1}{3} \right)} - (K_0' + 1) \left(\frac{V}{V_0} \right)^{-\left(\frac{(K_0'+1)}{3} \right)} \right] \qquad \text{---- } 2h$$

$$K_{T\,Tait} = K_0 \left(\frac{V}{V_0} \right) exp \left[(K_0' + 1) \left(1 - \frac{V}{V_0} \right) \right] \qquad \text{---- } 2i$$

$$K_{T\,Slater} = K_0 (K_0'' + 2) \left(\frac{V}{V_0} \right) - K_0 (K_0'' + 1) \left(\frac{V}{V_0} \right)^2 \qquad \text{---- } 2j$$

Pressure Derivative of Bulk Modudus K'_T
For Metals (Fe, Al And Cu)

$$K'_{T\,Birch-Mur.} = \frac{K_0}{3K_T}\left[\frac{3}{8}(K_0'-4)(81x^{-9}-98x^{-7}+25x^{-5})+\frac{1}{2}(49x^{-7}-25\,x^{-5})\right] \quad \text{----} 3a$$

$$K'_{T\,Bren.-Stacey} = \left(1-\frac{4}{3}\frac{P}{K_T}\right)\left(\left(K_0'-\frac{5}{3}\right)\frac{V}{V_0}+\frac{5}{3}\right)+\frac{16}{9}\frac{P}{K_T} \quad \text{----} 3b$$

$$K'_{T\,Shanker} = \left(1-\frac{4}{3}\frac{P}{K_T}\right)\left[\left(K_0'-\frac{8}{3}\right)\frac{V}{V_0}+\frac{8}{3}\right]+\frac{16}{9}\frac{P}{K_T} \quad \text{----} 3c$$

$$K'_{T\,Born} = \left(1-\frac{4}{3}\frac{P}{K_T}\right)K_0'+\frac{16}{9}\frac{P}{K_T} \quad \text{----} 3d$$

$$K'_{T\,Vinet} = \frac{1}{3}\left[\frac{x(1-x)+2\eta x^2}{1+(\eta x+1)(1-x)}+\eta x+2\right] \quad \text{----} 3e$$

$$K'_{T\,Hama-suito} = \frac{K_T}{P}+\frac{P}{9K_T}\left[x^2\left\{2\xi(1-x)-\frac{1}{(1-x)^2}\right\}+5\right]-\frac{1}{3} \quad \text{----} 3f$$

$$K'_{T\,Bardeen} = \frac{\left(8K_0'-\frac{88}{3}\right)-\left(25K_0'-\frac{250}{3}\right)\left(\frac{V}{V_0}\right)^{-1/3}+\left(18K_0'-54\right)\left(\frac{V}{V_0}\right)^{-2/3}}{\left(6K_0'-22\right)-\left(15K_0'-50\right)\left(\frac{V}{V_0}\right)^{-1/3}+\left(9K_0'-27\right)\left(\frac{V}{V_0}\right)^{-2/3}} \quad \text{----} 3g$$

$$K'_{T\,Ullmann} = \frac{\left(2K_0'-1\right)^2\left(\frac{V}{V_0}\right)^{\frac{(K_0'-2)}{3}}-\left(K_0'+1\right)^2}{3\left(2K_0'-1\right)\left(\frac{V}{V_0}\right)^{\frac{(K_0'-2)}{3}}-3\left(K_0'+1\right)} \quad \text{----} 3h$$

$$K'_{T\,Tait} = \left[\left(K_0'+1\right)\left(\frac{V}{V_0}\right)-1\right] \quad \text{----} 3i$$

$$K'_{T\,Slater} = \frac{2\left(K_0'+1\right)\left(\frac{V}{V_0}\right)-\left(K_0'+2\right)}{\left(K_0'+2\right)-\left(K_0'+1\right)\left(\frac{V}{V_0}\right)} \quad \text{----} 3j$$

Table 1. The theoretical values of input data K_T(GPa),K'_T&K_T"(GPa^{-1})

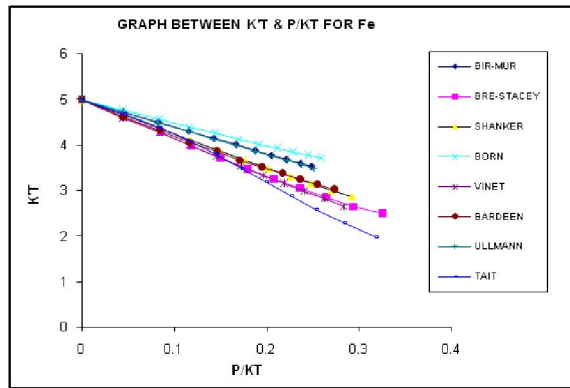| S.N0.	SOLIDS	K_T(GPa)	K'_T	K_T"(GPa^{-1})
1	Fe	170	4.98	-0.0851
2	Al	72.6	4.85	-0.104
3	Cu	135	5.93	-0.083

Results and Discussion

The value of Pressure P are computed with the help of equation ofpressure [eq.1a-1j] for Fe, Al and Cu at different compression using the values of Bulk modulus and its pressure derivatives at P=0 from Table-1. The results are shown in Fig-(1a, 2a 3a). The value of Bulk modulus and its pressure derivative are also computed at different pressure for Fe, Al and Cu using above equation -[2a-2j,3a-3j]. We have plotted the graph between P/K_T andK'_T are shown in Fig-(1b, 2b, 3b).
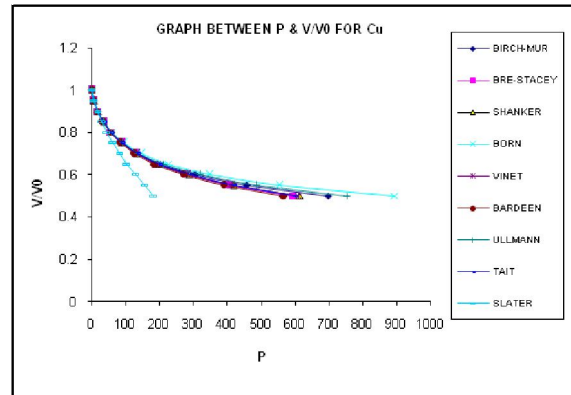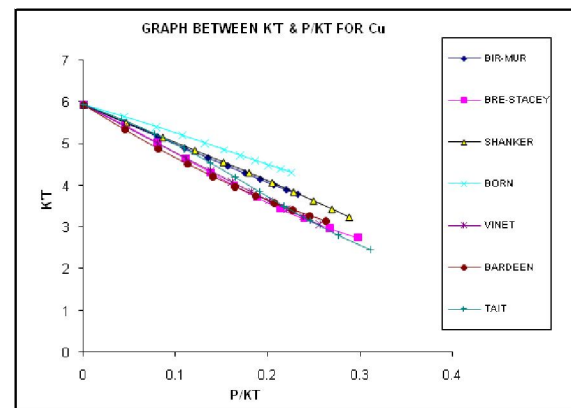
1. Graph for Metal - Fe :
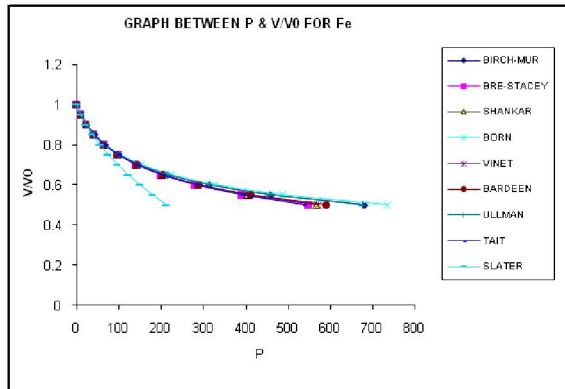
Fig1a: The Graph between P and V/V0
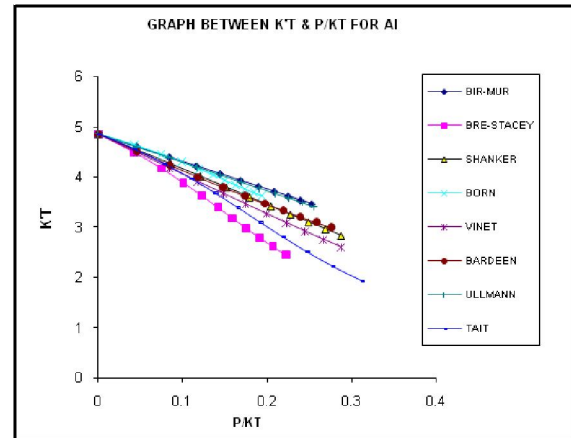
Fig-1b: The Graph between P/K_T and K'_T

2-Graph Formetal - Al

Fig 2a: The Graph between P and V/V0
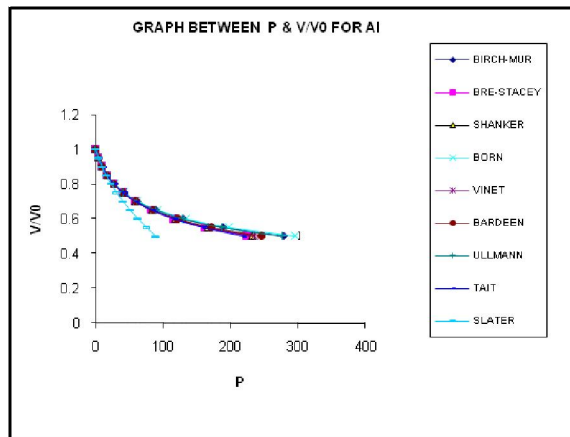
Fig 2b: The Graph between P/K_T and K'_T

3-   Graph Formetal - Cu

Fig 3a: The Graph between P and V/V0

Fig 3b: The Graph between P/K_T and K'_T

It is interesting to note from these Fig- (1b, 2b, 3b) that the limiting value of K'_T at finite pressure is varying from 3.0 to 3.5 instead of fix value 5/3. It has been claimed earlier that 5/3 is the limiting value of K'_∞ irrespective of any EOS. However the present study strongly suggests that it strongly depend upon the equation of state (EOS) because different EOS have been derived using different approach. Birch-Murnaghan[27], Bre-Stacey [29], Shanker [32], Hama-Suito [25], Vinet[30], and are showing satisfactory variation of pressure derivative of bulk modulus at infinite pressure in case of Fe, Al and Cu.

It is quite apparent from the Fig- (1b, 2b, 3b) that the value of K'_∞ for Fe, Al and Cu is nearly 3.0 which is higher than 1.6. Thus these metals even at extreme compression do not resemble with Thomas-Fermi electron gas. Hence the present study is useful in Geological and seismic studies in the earth's deep interior.

Conclusions

An EOS for metals provide useful information between Pressure (P), Bulk modulus(K_T) and Pressure derivative of bulk modulus (K'_T) which help us to understand the behaviour of the material under the effect of high pressure and high temperature.

EOS provides numerous information of non-linear compression of a material at high pressure and has been widely applied to engineering and other scientific researcher. Recently, rapid advances in computational techniques have extremely promoted the theoretical works. Significant progress has been achieved over the past year to describe the properties of condensed matter in terms of universal relationship involving a small number of parameters. The value of K'_∞ for Fe, Al and Cu is nearly 3.0 which is higher than 1.6. Thus these metals even at extreme compression do not resemble with Thomas- Fermi electron gas. Hence the present study is useful in Geological and seismic studies in the earth's deep interior. Further these EOS have been critically examined by evaluating the values of pressure derivative of bulk modulus at infinite pressure. The value of this parameter is found out to be grater than 5/3 by some EOS in case of Fe, Al and Cu such results is in good agreement with the Seismic Study of these metals.

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