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On pressure dependence of the relative compression (V/V_0) at room temperature for the solids : copper and lead as prototypes

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Abstract : A correction term has been introduced in the usual Tait's equation of state (EOS) and then used to predict the pressure dependence of the thermal compression for the solids : copper (Cu) and lead (Pb). The predictive capabilities of the complete EOS are discussed. The results obtained from the modified Usual Tait's equation of state are found closer to the available experimental data as compared to those values achieved without taking into account the correction factor in the original Tait's equation of state.

Keywords : Equation of relative compression, lead and copper, pressure dependence.

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There have been several studies to perform a universal model for the equation of state (EOS) of solids over the last decades. The fundamental importance of an equation of state provides not only a test to solid state theories derived from first principle, but also an easy way to calculate and to predict a variety of microscopic thermodynamical properties of a given solid .An analysis of volume compression in a solid at high pressure has been the subject of great interest [1-5] for its importance in understanding the microscopic behaviour of solids in physics and geophysics. It is also important to study prototypical systems in detail as a foundation for physical understanding in this rapidly expanding regime of experimentation. The metals like Cu and Pb are especially noteworthy for study in the 100-1000GPa range because of the fact that the *s-d* electron transfer can influence the properties of these materials, yet their position out side the normal transition metals in the periodic table, makes them more amenable to an accurate theoretical description.

Several studies on the equations of state based either on crystal potential [6, 7] or thermodynamic functions [8-12], have been performed in the past years. Among the number of isothermal EOS described earlier, we will refer to Vinet *et al* [13] and Usual Tait [14] equations of state because of their widespread use. A number of EOS's have been derived within the Mie-Gruneisen approximation in terms of the so-called cold pressure, and the temperature-dependence is introduced through thermal pressure [15, 16]. Taravillo *et al* [5] and Shanker *et al* [17] have recently investigated the phenomenological isothermal equation of state for solids and used them to study the compression behaviour of metals at room temperature. Taravillo *et al*'s equation of state is based on pseudo-spinodal assumption and Shanker's EOS is obtained from the lattice potential theory using the concept of short-range force constant as introduced by Born and Huang [18]. These equations are basically derived from Vinet EOS in terms of the binding energy of metals [19].

The main difficulty with the previous equations of state [5, 17] is that these EOS's require not only the more input parameters but also involve a heavy computational work to analyse the compression behaviour of solids at high pressure. On the other hand, Usual Tait's equation of state, however, requires less number of input parameter and provides a simple and straight forward approach to predict the relative compression in solids even at ultra high pressure. In spite of the wide application of Usual Tait's equation of state in the field of geophysics and condensed matter physics, this equation of state would, however, present the better results if a correction term of phonon pressure (P_{th}) is also included with the applied pressure, in the original Tait's equation of state. Since the phonon pressure as developed at high pressure (P) opposes the applied pressure, its sign must

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be taken negative with respect to the applied pressure. Here, we present a method of general validity for all types of solids which lead to the modified form of the Usual Tait EOS. The results based on the modified EOS are discussed and compared to the experimental data.

The original form of the Usual Tait equation (UTE) can be written as [14] :

(1)

where is the volume of the solid at the pressure required to compress it, keeping the temperature constant. V_0 is the initial value at $P = 0$ at room temperature T_0 .K_0 and K'_0 are the isothermal bulk modulus and its first pressure derivative at $T = T_0$.These parameters have been used in the present work as input data.

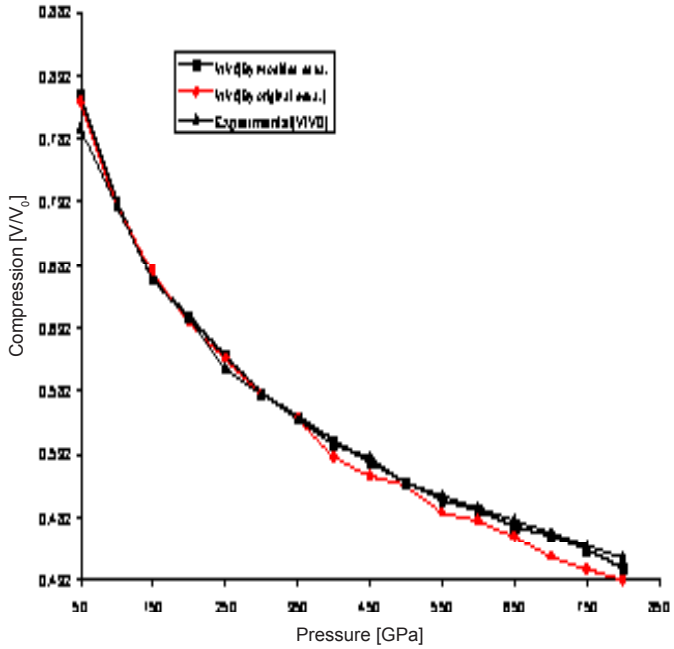

Figure 1. Shows the variation of relative compression (V/V_0) with pressure for the metal copper. Solid and continuous line represents our calculated results obtained from equation (2).

Including the effect of phonon pressure (P_{th}), in eq. (1), the original form of Usual Tait equation is modified as follows:

(2)

The thermal pressure (so-called phonon pressure) (P_{th}) can be evaluated from the following thermodynamical identity [20] :

(3)

Integration of eq. (3) gives

(4)

or

(5)

where the product of thermal expansion coefficient ( ) and isothermal bulk modulus (K_T) has been assumed to be constant at room temperature [8, 20]. The phonon pressure (P_{th}) calculated at reference temperature T_0 from eq. (5) has been subtracted from the each value of pressure as considered in present paper and then the eq. (2) has been used to analyse the compression behaviour of both metals copper and lead. The values of relative compression (V/V_0) as calculated from the modified eq. (2) are found in better agreement with the available experimental data as compared to those obtained from eq. (1).The values of relative compression (V/V_0) calculated for Cu and Pb from eqs. (1) and (2) are presented in Tables 1 and 2 respectively. The experimental values are also shown for the sake of comparison.

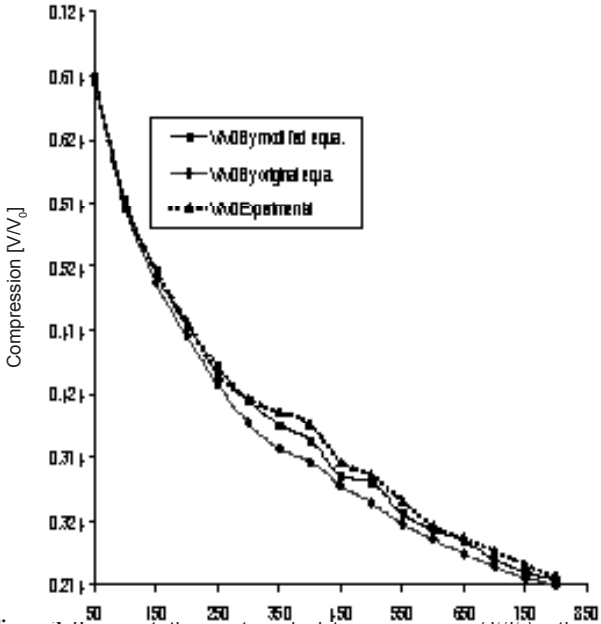

Figure 2. Represents the variation of relative compression (V/V_0) with pressure for lead.

We note from Tables 1 and 2 that the values of relative compression calculated from eq. (2) represent more close agreement with experimental data as compared to those obtained from eq. (1) originally known as Usual Tait equation of state (UTE). Introduction of the concept of the phonon pressure (P_{th}) in present study, thus improves not only the final results on compression properties but also provides the realistic approach to calculate the microscopic properties of the solid under the application of high pressure. A graphical presentation between the present calculated values and experimental data has also been shown.

Table 1. Calculated values of relative compression (V/V_0) with pressure for

Cu.

Pressure (Gpa) values	V/V_0 (a)*	(b)*	(c)*
50	0.816	0.811	0.790
100	0.733	0.730	0.730
150	0.670	0.678	0.670
200	0.641	0.637	0.640
250	0.610	0.608	0.600
300	0.580	0.580	0.580
350	0.562	0.561	0.560
400	0.543	0.530	0.540
450	0.526	0.515	0.530
500	0.510	0.508	0.510
550	0.496	0.486	0.500
600	0.488	0.480	0.490
650	0.475	0.467	0.480
700	0.468	0.451	0.470
750	0.456	0.441	0.460
800	0.442	0.432	0.450

(a) Calculated from the modified equation of state (2).
(b) Calculated from the original equation of state (1).
(c) Experimental values [5].

Table 2. Calculated values of relative compression (V/Vo) with pressure for Pb.

Pressure (GPa) values	V/V_0 (a)*	(b)*	(c)*
50	0.673	0.670	0.670
100	0.578	0.572	0.570
150	0.520	0.512	0.520
200	0.478	0.470	0.480
250	0.446	0.432	0.440
300	0.419	0.401	0.420
350	0.400	0.381	0.410
400	0.387	0.370	0.400
450	0.360	0.352	0.370
500	0.354	0.338	0.360
550	0.330	0.322	0.340
600	0.317	0.310	0.320
650	0.309	0.298	0.310
700	0.294	0.288	0.300
750	0.284	0.280	0.290
800	0.278	0.274	0.280

(a) Calculated from the modified equation of state (2).
(b) Calculated from the original equation of state(1).
(c) Experimental values[5].

In the present study, we have thus made an attempt to modify the UTE in view of the theory of phonon pressure and predicted the more correct values of relative compression for the solids Cu and Pb. It is further found that the modified form of the equation of state [eq. (2)] can also be used for studying the high pressure physics of more complex solids irrespective of their structure.

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