Available online at www.elixirpublishers.com (Elixir International Journal)

Crystal Research Technology

Elixir Crystal Research Tech. 42 (2012) 6299-6305

Equation of state for superconductors based on finite strain theory under high

pressure

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Article history: Received: 29 October 2011; Received in revised form: 2 January 2012; Accepted: 13 January 2012;

Keywords Finite strain, Superconductors, EOS, Eulerian strain, Hencky strain.

ABSTRACT

We have reformulated equations of state (EOS) for superconductors based on Lagrangian and Eulerian strains following the method developed by Stacey. The expressions thus obtained are used conveniently to assess the validity of various EOS for different types of superconductors. The logarithmic EOS based on the Hencky measure of finite-strain is also modified by including the higher terms arising from the fourth-order contribution in the Taylor series expansion of the free energy. In the present work, pressure of five different superconductors viz. YBa2Cu3O6.6, YBa2Cu3O6.93, YBa2Cu3O7, Bi2Sr2CaCu2O8 and Nd1.32Sr0.41Ce0.27CuO3.96 has been computed at different compression ranges using five different EOS based on finite strain theory viz. Third order Eulerian EOS, Third order Lagrangian EOS, Second order Born-Mie EOS, Third order Born-Mie EOS and Bardeen EOS. the obtained results are compared with available experimental data to test the validity and success of these equation of states.

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Introduction

The application of single-crystal X-ray diffraction techniques to several specimens that are being compressed within a single, hydrostatic pressure chamber offers a precise method for determining the relative compressibility's of different crystals [1-4]. In this way, it is possible to resolve the effects on the equation of state of varying composition, nonstoichiometry, site disordering, or other subtle factors. Hence, the finite-strain theory of equations of state has been extended to the analysis of such data [5-7].

The purpose of this paper is to illustrate the finite-strain analysis of relative compressibility by applying it to the recently published data for the high-pressure superconducting phase. In geophysics and high-pressure research, experimental or theoretical data consisting of pressure, temperature, and volume triplets PVT are parameterized to a functional form for ease of interpolation and extrapolation. These equations of state are then used to compute phase diagrams, or are used in geodynamic or shock compression modeling, etc. [8], comprehensively reviews equation-of-state formulations, and comprehensive reviews and comparisons of equations of state are given by Hama and Suito[9], Stacey [10], and Duffy and Wang [11]. The primary purpose of this paper is to discuss the reasons for the accuracy of the most-used formulation, based on finite strain theory and experimental compare with the available data for superconductors. Here we show that at high compressions, and for highly compressible materials the third order Birch Murnaghan equation of state is considerably more accurate. The above equations of state are appropriate for isothermal data. To include thermal expansivity there are main approaches to fit isotherms, and then tabulate or fit the parameters V0, K0, and K0'as functions of temperature. Since experimental data are not always collected along isotherms, that method is most amenable to analysis of theoretical results.

The equation of state (EOS) is fundamentally important in studying the high pressure properties of solids, which causes structural transition. The importance of high pressure investigations for high TC superconductors was recognized after the discovery of superconductivity at 30K in La-Ba-Cu-O system by Bednorz and Muller [12]. The superconducting transition temperature of this system increases by 10K under the pressure of 15Kbar, which was not observed in any known superconductors [13]. In fact this led to the successful idea of replacing La by smaller Y, resulting to YBa2Cu3O7 superconductors [14] with Tc at 90K.

Since the discovery of the high-temperature superconductors, there have been an enormous number of studies designed to increase the critical temperature and to provide an understanding of the mechanical responsible for superconductivity. It has been conformed that, in the mineral YBa2Cu3O7, a single phase YBa₂Cu₃O_{9-x} ($x\approx 2$) is responsible for the high transition temperature. Borges *et a* [15] observed that pressure has a positive effect on superconducting transition temperature (Tc) and is enhanced at a rate of about 0.09 K/kbar for YBa₂Cu₃O₆ and 0.19 K/kbar for YbBa₂Cu₃O_x.

In order to test equation-of-state formulations, it is important to study large compressions, because most common equations of state will work reasonably over small compression ranges. Thus we choose to study the very compressible superconducting materials $YBa_2Cu_3O_{6.6}, YBa_2Cu_3O_{6.93},$ $YBa_2Cu_3O_7$, $Bi_2Sr_2CaCu_2O_8$ and $Nd_{1.32}Sr_{0.41}Ce_{0.27}CuO_{3.96}$. The results turn out to be significant, not only as an illustrative example but also because they address empirical conclusions that have been emerging from research in Geophysics and condensed matter physics.

Theoretical

Finite-strain theory has been applied extensively to problems in geophysics. The resulting equations are called semi



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(2)

empirical because they contain parameters that have to be determined from experiment. The theory relates strain, or compression, to pressure.

It is well known result [16,17] of continuum mechanics that the finite strain theory may be written equivalently in terms of any of an infinite number of different definitions of the 'strain'. For the case of an elastic solid (i.e. one possessing a free energy function which is uniquely defined in terms of deformation and temperature), this result implies, specifically, that the stressstrain relation may be written equivalently in an infinite number of ways.

$$R-R_0 \equiv eR_0 \tag{1}$$

$$\sigma = (1+e) \left(\frac{\partial F}{\partial \eta}\right)_{T} (1+e) \frac{1}{V}$$

Here R is a vector to a point in the deformed lattice; R_0 is the vector to the same point in the undeformed reference state, denoted in this section by a subscript zero. The components of both are referred to the same set of cartesian axes. e is the finite strain tensor defined by equation (1). σ is the homogeneous stress at the point R. 1 is the unit 3×3 tensor. $(1)_{ij}=\delta_{ij}$. F is the Helmholtz free energy, or 'elastic energy' function. η is the symmetric finite strain tensor defined in relation to e by $\eta_{ii} = (1/2)(e_{ii}+e_{ii}+e_{mi}e_{mi})$ (3)

Equation (2) is exact, i.e. independent of the size of e. It is derived by Leibfried and Ludwig [18] and Murnaghan [19]. Alternatively, the strain f can be defined implicitly by

$$\mathbf{R} - \mathbf{R}_0 = \mathbf{f} \, \mathbf{R} \tag{4}$$

And then the stress-strain relation is

$$\sigma = \left(1 - 2\varepsilon\right) \left(\frac{\partial F}{\partial \varepsilon}\right)_{T} \frac{1}{V}$$
⁽⁵⁾

Where the symmetric tensor ε defined in relation to f by

$$\varepsilon_{ij} = (1/2)(f_{ij} + f_{ji} - f_{mj}f_{mi})$$

Equation (5) is also exact, though its generality is restricted to special situations, including the important cases of isotropic bodies and of pure strains unaccompanied by rotations [20]. The relations between strain and volume change is: $(V/V_0)^2 = |\det(1+2\eta)|$ (7)

$$(V_0/V)^2 = |\det(1 - \varepsilon)| \tag{8}$$

V is specific volume and V_0 is volume at zero pressure.

The difference between these two definitions of strain given by equation (1) and equation (4) is clearly in the selection of the characteristic lengths used as coefficients of the strain. In the first case, the characteristic lengths are taken from the reference state where as in the second, from the deformed state. Because of this essential difference, the strains e and η are called 'Lagrangian' or 'material' definitions of strain, the strain f and ϵ are called 'Eulerian' or 'spatial' definitions of strain. An elegant and exhaustive discussion of finite strain has been given by Truesdell [16].

Although equations (2) and equation (5) are exact, there usefulness is limited by the need for expressions for the free energy as a function of strain. In general, the physical description of the free energy in terms of interatomic forces, etc.will imposes requirements on the choice of a definition of strain [21].

Also, any approximations made in F will affect the results of the choice of a definition of strain. Hence, the application of equations (2) and (5) to real solids will not be exact and further will depend critically upon choice of definition of strain. Different choices lead to non equivalent equations of state. Eulerian and Hencky measures of strain

The commonly used Eulerian measure of finite strain is based on the consideration of the distance element ds² and on the analysis of its change during deformation, the final deformed state being the reference state. The result is usually expressed in terms of displacement field u_i as [22,23]

$$\left(\mathbf{e}_{\mathrm{E}}\right)_{ij} = \frac{1}{2} \left[\frac{\partial \mathbf{U}_{i}}{\partial \mathbf{x}_{j}} + \frac{\partial \mathbf{U}_{j}}{\partial \mathbf{x}_{i}} - \frac{\partial \mathbf{U}_{k}}{\partial \mathbf{x}_{j}} \frac{\partial \mathbf{U}_{k}}{\partial \mathbf{x}_{i}} \right]$$
(9)

Hydrostatic pressure produces an isotropic (negative) compressional Eulerian strain $\varepsilon_{\rm E}$ [24], which can be written as

$$\varepsilon_{\rm E} = \frac{1}{2} \left| 1 - \left(\frac{V_0}{V} \right)^{2/3} \right| \tag{10}$$

The Lagrangian strain, ε_L referred to the initial sate is

$$\varepsilon_{\rm L} = \frac{1}{2} \left[\left(\frac{\rm V}{\rm V_0} \right)^{2/3} - 1 \right] \tag{11}$$

It may be noticed that if V goes to zero (i.e., for very large compressions), the langrangian strain tends to find the value -1/2, which makes its use in appropriate at high pressure.

Structural geologists and materials scientists use a different definition of strain [25, 26]. The reference state is neither the initial nor the final configuration, but the instantaneous configuration of the body being deformed. In uniaxial deformation, as the instantaneous length 1 of the body is increased by an infinitesimally small increment dl, the ratio dl/l is considered as an increment of the current state of strain

$$d\varepsilon = \frac{dl}{l}$$
(12)

When the body goes from length l_0 to length 1 the total finite strain or natural strain, also called the Hencky measure of strains [27-29], is obtained by integration,

$$\varepsilon_{\rm H} = \int_{l_0}^{l} d\varepsilon = \int_{l_0}^{l} \frac{dl}{l} = \ln \frac{1}{l_0}$$
(13)

The Hencky strain is not generally used because the integration is considered possible only when the increment principal axes do not rotate during the deformation Malvern [29]. As this is the case for deformation under hydrostatic pressure [30], we can write

$$\varepsilon_{\rm H} = \frac{1}{3} \ln \frac{\rm V}{\rm V_0} \tag{14}$$

Equation of state

The practical expression for Finite strain were developed by Birch [31,32]. The classical theory of infinitesimal elasticity is based on two assumptions:

(1). The strains are uniquely determined by stresses and are reversible.

(2). The strains are limited to linear elasticity.

Birch used Murnaghan's basic theory, but restricted it to the case where the initial stress is a large hydrostatic pressure. The crucial assumption in finite strain theory is in the formal relationship between compressions and co-ordinate displacement [33], one form is

$$\frac{V}{V_0} = \eta = (1 + 2\epsilon)^{3/2}$$
(15)

where ε is strain. The relation ship between η and ε is not unique. Another alternative is [34]

$$\eta = (1 - 2\varepsilon)^{-3/2} \tag{16}$$

Equation (15) is Lagrangian formulations where as (16) is Eulerian formulation.

A series in strain (ϵ) for the energy function

A simple relationship between the compression η and strain variable [34] is given by

 $\varepsilon = f(\eta)$

Let the symbol ε' denote $d\varepsilon/dv$, $\varepsilon''=d^2\varepsilon/dv^2$ etc. Take the expansion in the potential as a Taylor's series in the equation

$$\mathbf{E}(\boldsymbol{\varepsilon}) = \mathbf{K}_{\mathrm{T0}} \mathbf{V}_{0} \sum_{\mathbf{P}=2}^{\infty} \left(\frac{\mathbf{C}_{\mathbf{P}}}{\mathbf{P}!} \right) \boldsymbol{\varepsilon}^{\mathbf{P}}$$
(17)

where P denotes a power. The condition P(1)=P₀=0 is satisfied by ignoring the term P=1 the factor $K_{T0}V_0$ has the dimensions of energy so that all coefficients C_P and ε are dimensionless. Further E'=P where E' = $(\partial E/\partial V)_T$ Further

Eurther E = P where E =
$$(\partial E/\partial V)_{T}$$
, Further
E'' = $-(K/V)$ (18)
 $E^{'''} = -\frac{K}{V^2} \left(\frac{VK'}{K} + 1\right)$ (19)

The derivatives of equation (17) is

$$E' = K_{T_0} V_0 \mathscr{E}' C_2 \left\{ 1 + \sum_{P=3} \frac{C_P}{C_2} \left[\frac{\mathscr{E}^{P-2}}{(P-1)!} \right] \right\}$$
(20)

$$E^{''} = K_{T_0} V_0 C_2 \left(\left(\varepsilon \cdot \varepsilon' + \varepsilon \cdot \varepsilon' \right) + \sum_{P=3} \frac{C_P}{C_2} \left[\left\{ \frac{\varepsilon \cdot \varepsilon'}{(P-2)!} + \frac{\varepsilon' \cdot \varepsilon}{(P-1)!} \right\} \right] \varepsilon^{P-2} \right)$$
(21)

$$E^{"} = K_{T0}V_0C_2 \left[3\varepsilon'\varepsilon''\sum_{P=3} \frac{C_P}{C_2} \left\{ \left[\frac{\varepsilon'\varepsilon'\varepsilon'}{(P-3)!} + \frac{3\varepsilon'\varepsilon''}{(P-2)!} + \frac{\varepsilon'''\varepsilon^2}{(P-1)!} \right] \right\} \varepsilon^{(P-3)} \right] (22)$$

For P=0, $\epsilon = \epsilon_0 = 0$

since Then

$$E'' = K_T / V$$
$$E_0'' = (K_T / V_0)$$

Another expression for E_0 " is found from equation (21) for n=2 and ε_0 =0 the terms behind the summation sign in equation (21) vanishes& E_0 " becomes

$$\mathbf{E}_{0}^{''} = \mathbf{K}_{\mathrm{T0}} \mathbf{C}_{2} \mathbf{V}_{0} \left(\boldsymbol{\varepsilon}_{0}^{'} \right)^{2}$$
(24)

From equation (23) and equation (24)

$$C_2 = \frac{1}{\left(V_0 \varepsilon_0^{\prime}\right)^2} \tag{25}$$

Similarly where

$$\mathbf{K}_{0} = \left(\frac{\partial \mathbf{K}_{\mathrm{T}}}{\partial \mathbf{P}}\right)_{\mathrm{T}}$$
 at $\mathbf{P}=0$

For n=3 & $\varepsilon_0=0$, the $\varepsilon\varepsilon''' \varepsilon^2$ term in equation (22) vanishes and all but the $(\varepsilon')^3$ term behind the summation sign in equation (22) vanish leaving

$$E_{0}^{""} = K_{T0}V_{0}C_{2}\left[3\varepsilon_{0}^{'}\varepsilon_{0}^{"} + \frac{1}{2}C_{3}\left(\varepsilon_{0}^{'}\right)^{3}\right]$$
(26)

Equating equation (25) and equation (26), C₃ becomes

$$C_{3} = -\left[\frac{\left(1 - K_{0}\right)}{\left(\varepsilon_{0}V_{0}\right)^{3}} + \frac{3C_{2}\varepsilon_{o}}{\left(\varepsilon_{0}\right)^{2}}\right]$$
(27)

The pressure equation to third order is

$$\mathbf{P} = \mathbf{E}' = \mathbf{K}_{T0} \mathbf{V}_0 \boldsymbol{\varepsilon} \boldsymbol{\varepsilon}' \left(\mathbf{C}_2 + \frac{1}{2} \mathbf{C}_3 \boldsymbol{\varepsilon} \right)$$
$$= \frac{\mathbf{K}_{T0} \mathbf{V}_0 \boldsymbol{\varepsilon} \boldsymbol{\varepsilon}'}{(\boldsymbol{\varepsilon}_0 \mathbf{V}_0)^2} \left\{ 1 - \frac{\boldsymbol{\varepsilon}}{2} \left(\frac{1 + \mathbf{K}_0'}{\boldsymbol{\varepsilon}_0' \mathbf{V}_0} + \frac{3\boldsymbol{\varepsilon}_0''}{(\boldsymbol{\varepsilon}_0')^2} \right) \right\}$$
(28)
The energy equation for third order is

The energy equation for third order is

$$E(\varepsilon) = \frac{1}{2} K_{T0} V_0 E^2 \left(C_2 + \frac{1}{3} C_3 \varepsilon \right)$$

$$= \frac{1}{2} K_{T0} V_0 \varepsilon^2 \left\{ \frac{1}{(\varepsilon_0^{'} V_0)^2} - \frac{\varepsilon}{3} \left[\frac{1 + K_0^{'}}{\varepsilon_0 V_0^3} + \frac{3}{(\varepsilon_0 V_0)^3} \frac{\varepsilon_0^{''}}{(\varepsilon_0^{'})^2} \right] \right\}$$

$$= \frac{1}{2} \frac{K_{T0} V_0 \varepsilon^2}{(\varepsilon^{'} V_0)^2} \left\{ 1 - \frac{\varepsilon}{3} \left[\frac{1 + K_0^{'}}{\varepsilon_0 V_0} + \frac{3\varepsilon_0}{(\varepsilon_0^{'})^2} \right] \right\}$$
(29)

Equation of state based on Eulerian Strain The Eulerian strain for

$$\varepsilon(\eta) = \frac{1}{2}(1 - \eta^{-2/3}) = \left(\frac{1}{2}\right) \left[1 - \left(\frac{V_0}{V}\right)^{2/3}\right]$$
(30)

we have

(23)

$$\varepsilon' = \frac{1}{3V_0} \eta^{-5/3}$$
 $\varepsilon'_0 = \frac{1}{3V_0}$ (31a)

$$\varepsilon'' = -\frac{5}{9V_0^2} \eta^{-8/3} \qquad \varepsilon''_0 = -\frac{5}{9V_0^2}$$
(31b)

$$\frac{\varepsilon'}{\varepsilon_0} = \eta^{-5/3} \qquad \qquad \frac{\varepsilon_0}{(\varepsilon_0')^2} = -5 \qquad (31c)$$

$$\varepsilon^{'''} = \frac{40}{27} \frac{1}{V_0^3} \eta^{-11/3} \qquad \frac{\varepsilon_0^{'''}}{(\varepsilon_0)^3} = 40$$
 (31d)

where $\epsilon' = (\partial \epsilon / \partial V)$ and $\epsilon'' = (\partial \epsilon' / \partial v)$

Now from equations (27), (31a), (31b) and (31c) the third order coefficient can be written as

$$C_3 = -27(K_0' - 4)$$

Thus, from equation (29) the third order in Eulerian strain Energy (at T=0)

$$\mathbf{E}(\varepsilon) = \mathbf{U} - \mathbf{E}_{\rm ST} = \frac{9}{2} \mathbf{K}_{\rm T0} \mathbf{V}_0 \varepsilon^2 \left[1 - \frac{3}{2} (\mathbf{K}_0^{\prime} - 4) \varepsilon \right]$$
(32)

and the EOS is

$$P(\varepsilon, 0) = -3K_{T0}(1 - 2\varepsilon)^{-5/2} \varepsilon \left[1 - \frac{3}{2} (K_0' - 4)\varepsilon \right]$$
(33)

Equation of state based on Lagrangian Strain The Lagrangian strain is given by

$$\varepsilon = \frac{1}{2} \left(\eta^{2/3} - 1 \right) = \frac{1}{2} \left[\left(\frac{V}{V_0} \right)^{2/3} - 1 \right]$$
$$\varepsilon' = \frac{1}{3V_0} \eta^{-1/3} \qquad \varepsilon'' = -\frac{1}{9V_0^2} \eta^{-4/3} \qquad \frac{\varepsilon}{\varepsilon_0} = \eta^{-1/3}$$

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Now from equation (28) the pressure equation for third order is

$$\mathbf{P} = \mathbf{K}_{\mathrm{T0}} \mathbf{V}_{0} \boldsymbol{\varepsilon} \boldsymbol{\varepsilon}' \left(\mathbf{C}_{2} + \frac{1}{2} \mathbf{C}_{3} \boldsymbol{\varepsilon} \right)$$

where

$$C_2 = \frac{1}{(V_0 \varepsilon_0)^2} = 9$$

and

$$C_{3} = -\left[\frac{1}{(V_{0}\varepsilon_{0}^{'})^{3}}\left(1 - K_{0}^{'}\right) + \frac{\varepsilon_{0}^{'} 3C_{2}}{(\varepsilon_{0}^{'})^{2}}\right] = -27K_{0}^{'}$$

using above, the EOS in third order

$$P(\varepsilon,0) = -9K_{T0}V_{0}\varepsilon\varepsilon(1-3K_{0}\varepsilon)$$
(34)

In terms of compression η it is [35]

$$P(\eta,0) = -\frac{3}{2}K_{T0}\left(\eta^{1/3} - \eta^{-1/3}\right)\left[1 - \frac{3}{4}K_{0}(\eta^{2/3} - 1)\right] \quad (35)$$

Birch - Murnaghan Isothermal Equation of state

Birch original derivations were based on Murnaghan's theory of finite elasticity. The EOS presented by Birch in terms of parameter ε is Birch original derivations were based on Murnaghan's theory of finite elasticity. The EOS presented by Birch in terms of parameter ε is

$$\varepsilon = \frac{3}{4} \left(4 - \mathbf{K}_{0}^{'} \right)$$

In terms of the compression η and the experimentally determined K_{T0} and $K_0^{'}$ the isothermal B-M EOS to second order is

$$P(\eta,0) = \frac{3}{2} K_{T0} \left(\eta^{-7/3} - \eta^{-5/3} \right)$$
(36)

Isothermal B-M equation of state to the third order

$$P(\eta,0) = (-3/2)K_{T0}(\eta^{-5/3} - \eta^{-7/3})[1 - (3/4)(K_0^{-4})(1 - \eta^{-2/3})]$$
(37)

The Bardeen EOS

Bardeen's EOS arises from an assumption of an interatomic potential between atoms. The potential function is given by $\Phi(r)=A(r_0/r)+B(r_0/r)^2+C(r_0/r)^3$ (38)

The strain function appropriate to Bardeen potential is $\epsilon(\eta)=[1-(V_0/V)^{1/3}]=(1-\eta^{-1/3})$ (39) Using this the second order Bardeen EOS

 $P(\eta, 0) = -3K_{T0}(\eta^{-5/3} - \eta^{-4/3})$ (40) The Third order Bardeen EOS is

$$P(\eta, 0) = -3K_{T0}(\eta^{-4/3} - \eta^{-5/3})[1 - (3/2)(K_0' - 3)(1 - \eta^{-1/3})]$$
(41)

Results and Discussion

The variation of pressure with unit cell volume of five high temperature superconductors viz. $YBa_2Cu_3O_{6.6}$, $YBa_2Cu_3O_{6.93}$, $YBa_2Cu_3O_7$, $Bi_2Sr_2CaCu_2O_8$, $Nd_{1.32}Sr_{0.41}Ce_{0.27}CuO_{3.96}$ have been computed by using third order Eulerian EOS (P1), third order Lagrangian EOS (P2), second order B-M EOS (P3), third order B-M EOS (P4) and Bardeen EOS (P5) and compared with their experimental values [36-39]. The values of isothermal bulk modulus (K₀) and its first pressure derivative (K₀) at zero pressure are for these superconductors are used as input parameter, given in table (1) which are obtained from neutron diffraction measurements methods, taken from the literature [39-

42]. The values of pressure computed by using equations (33), (35), (36), (37) and (41) at different compressions with their percentage deviation from experimental values are listed in tables (2-6). It is evident from the table (2-6) that the third order Lagrangian and third order Birch-Murnaghan EOS give the best agreement with experimental values. The maximum deviation from experimental values is only up to 3.67 %. It is also observed from the tables that compression values upto the 0.995, calculated values of pressure for five EOS are almost same as experimental values for all the superconductors, but as the compression increases after 0.995, the deviation in values of pressure increases. The second order Birch-Murnaghan EOS yields poor results at increased compressions. The order of superiority can be arranged as follows on the basis of EOS used in present study for the calculation of pressure at different compressions for superconductors.

It is crystal clear from table (2-6) that the compounds with larger value of oxygen content (δ) value is more compressible, in agreement with experimental observation.

The study of Gravari et al. [38] for $Bi_2Sr_2CaCu_2O_8$ at pressure 0 and 10 kbar, V/V0=0.985 is in good agreement with the present approach. A neutron diffraction study of compression performed by Izumi et al. [39] for Nd_{1.32}Sr_{0.41}Ce_{0.27}CuO_{3.96}. They have studied for variation of unit cell volume at different pressure varying form 0 to 0.637GPa. The result thus obtained by Izumi are compared with the calculated value of pressure computed by third order Lagrangian EOS and third order Bardeen EOS.

The results shows an excellent agreement with maximum percentage deviation of 2.31% at $V/V_0=0.990$. The experimental value of pressure at high compressions could not available. More generally Anderson OL [8] and Stacey et al. [10] note that second order Birch Murnaghan equation is subjected to a truncation problem due to the fact that the coefficient of the term of degree 2 of the polynomial expansion of the free energy is larger than that of the degree 3 leading to bad convergence for large strains. Due to this shortcomings the second order Birch Murnaghan equation of state fails hopelessly.

When the finite strain is defined by the change in distance between two neighbouring points during deformation, the problem arises of choosing between the Eulerian and Lagrangian schemes. Now the Lagrangian and Eulerian strains behave very different for large extension and compression and are equivalent only for small strains.

The essential difference between the two kinds of strain is that the Lagrangian approach uses the original and unstrained state as the reference, whereas, the Eulerian approach uses the deformed state as the reference.

It is easily seen from equation (30) and (30a) that for infinite extension $(V \rightarrow \infty)$ the Eulerian strain takes the finite value (1/2) while for infinite compression $(V \rightarrow \infty)$ the Lagrangian strain takes the finite value (-1/2). This obviously makes the Lagrangian strain is most suitable for large compression.

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Table-1 Input values of isothermal bulk modulus (K_0) and its first pressure derivative (K_0) at zero pressure

	for Superconductors										
S.No	Superconductors	K ₀ (GPa)	K ₀								
1	YBa ₂ Cu ₃ O _{6.6}	112	5.16								
2	YBa2Cu3O6.93	123	5.16								
3	YBa ₂ Cu ₃ O ₇	150	5.15								
4	Bi ₂ Sr ₂ CaCu ₂ O ₈	61	5.16								
5	Nd _{1.32} Sr _{0.41} Ce _{0.27} CuO _{3.96}	143	5.18								

	corresponding percentage deviation													
V/V ₀	$\Delta P(1)$ % div.	P(1)	$\Delta P(1)$ % div.	P(2)	$\Delta P(1) \%$ div.	P(3)	$\Delta P(1)$ % div.	P(4)	$\Delta P(5)$ % div.	P(5)	P(exp)			
1.000		0.00		0.00		0.00		0.00		0.00	0.00			
0.999	0.00	0.11	0.00	0.11	0.00	0.11	0.00	0.11	0.00	0.11	0.11			
0.998	0.00	0.23	0.00	0.23	0.00	0.23	0.00	0.23	0.00	0.23	0.23			
0.997	0.00	0.34	0.00	0.34	0.00	0.34	0.00	0.34	0.00	0.34	0.34			
0.996	0.00	0.45	0.00	0.45	0.00	0.45	0.00	0.45	0.00	0.45	0.45			
0.995	0.00	0.57	0.00	0.57	0.00	0.57	0.00	0.57	0.00	0.57	0.57			
0.990	0.00	1.15	0.87	1.16	0.00	1.15	0.87	1.16	0.87	1.16	1.15			
0.985	1.12	1.76	1.12	1.76	2.25	1.74	1.12	1.76	1.12	1.76	1.78			
0.980	0.83	2.38	0.83	2.38	1.67	2.36	0.83	2.38	0.83	2.38	2.40			
0.970	0.54	3.68	0.27	3.69	1.89	3.63	0.27	3.69	0.27	3.69	3.70			
0.960	0.98	5.05	0.39	5.08	2.75	4.96	0.39	5.08	0.39	5.08	5.10			
0.950	1.67	6.49	0.61	6.56	3.48	6.37	0.61	6.56	0.76	6.55	6.60			
0.940	1.11	8.01	0.37	8.13	3.21	7.84	0.37	8.13	0.25	8.12	8.10			

Table – 2: Comparison of Variation of pressure P (in GPa) versus unit cell volume ratio (V/V₀) calculated by (1) Third degree Eulerian EOS (2) Third degree Lagrangian EOS (3) Second order B-M EOS (4) Third order B-M EOS (5) Bardeen EOS with experimental value for YBa₂Cu₃O_{6.6} with corresponding percentage deviation

Table – 3: Comparison of Variation of pressure P (in GPa) versus unit cell volume ratio (V/V₀) calculated by (1) Third degree Eulerian EOS (2) Third degree Lagrangian EOS (3) Second order B-M EOS (4) Third order B-M EOS (5) Bardeen EOS with experimental value for YBa₂Cu₃O_{6.93} with corresponding percentage deviation with experimental values

V/V ₀	P (1)	$\Delta P(1)$ % div.	P(2)	$\Delta P(2)$ % div.	P(3)	$\Delta P(3)$ % div.	P(4)	$\Delta P(4)$ % div.	P(5)	$\Delta P(5)$ % div.	P(exp)
1.000	0.00		0.00		0.00		0.00		0.00		0.00
0.999	0.12	0.00	0.12	0.00	0.12	0.00	0.12	0.00	0.12	0.00	0.12
0.998	0.25	0.00	0.25	0.00	0.25	0.00	0.25	0.00	0.25	0.00	0.25
0.997	0.37	0.00	0.37	0.00	0.37	0.00	0.37	0.00	0.37	0.00	0.37
0.996	0.50	0.00	0.50	0.00	0.50	0.00	0.50	0.00	0.50	0.00	0.50
0.995	0.62	0.00	0.62	0.00	0.62	0.00	0.62	0.00	0.62	0.00	0.62
0.990	1.27	2.31	1.27	2.31	1.26	3.08	1.27	2.31	1.27	2.31	1.30
0.985	1.93	1.58	1.93	1.58	1.92	1.05	1.93	1.58	1.93	1.58	1.90
0.980	2.61	0.38	2.62	0.77	2.59	0.38	2.62	0.77	2.62	0.77	2.60
0.970	4.04	0.50	4.05	0.75	3.98	1.00	4.05	0.75	4.05	0.75	4.02
0.960	5.54	1.07	5.58	0.36	5.45	2.68	5.58	0.36	5.58	0.36	5.60
0.950	7.13	0.97	7.20	0.00	6.99	2.92	7.20	0.00	7.19	0.14	7.20
0.940	8.80	1.12	8.93	0.34	8.61	3.26	8.93	0.34	8.91	0.11	8.90

	percentage deviation with experimental values												
V/V ₀	P (1)	$\Delta P(1)$ % div.	P(2)	$\Delta P(2)$ % div.	P(3)	$\Delta P(3)$ % div.	P(4)	$\Delta P(4)$ % div.	P(5)	$\Delta P(5)$ % div.	P(exp)		
1.000	0.00		0.00		0.00		0.00		0.00		0.00		
0.999	0.15	0.00	0.15	0.00	0.15	0.00	0.15	0.00	0.15	0.00	0.15		
0.998	0.30	0.00	0.30	0.00	0.30	0.00	0.30	0.00	0.30	0.00	0.30		
0.997	0.45	0.00	0.45	0.00	0.45	0.00	0.45	0.00	0.45	0.00	0.45		
0.996	0.61	0.00	0.61	0.00	0.61	0.00	0.61	0.00	0.61	0.00	0.61		
0.995	0.76	0.00	0.76	0.00	0.76	0.00	0.76	0.00	0.76	0.00	0.76		
0.990	1.55	1.97	1.55	1.97	1.54	1.32	1.55	1.97	1.55	1.97	1.52		
0.985	2.35	0.86	2.36	1.29	2.34	0.43	2.36	1.29	2.36	1.29	2.33		
0.980	3.19	0.31	3.19	0.31	3.16	1.25	3.19	0.31	3.19	0.31	3.20		
0.970	4.92	0.20	4.94	0.61	4.86	1.02	4.94	0.61	4.94	0.61	4.91		
0.960	6.76	0.59	6.80	0.00	6.64	2.35	6.80	0.00	6.80	0.00	6.80		
0.950	8.69	1.14	8.78	0.11	8.53	2.96	8.78	0.11	8.77	0.23	8.79		
0.940	10.73	1.56	10.89	0.09	10.50	3.67	10.89	0.09	10.87	0.28	10.90		

Table – 4: Comparison of Variation of pressure P (in GPa) versus unit cell volume ratio (V/V₀) calculated by (1) Third degree Eulerian EOS (2) Third degree Lagrangian EOS (3) Second order B-M EOS (4) Third order B-M EOS (5) Bardeen EOS with experimental value for YBa₂Cu₃O₇ with corresponding percentage deviation with experimental values

Table – 5: Comparison of Variation of pressure P (in GPa) versus unit cell volume ratio (V/V₀) calculated by (1) Third degree Eulerian EOS (2) Third degree Lagrangian EOS (3) Second order B-M EOS (4) Third order B-M EOS (5) Bardeen EOS with experimental value for Bi₂Sr₂CaCu₂O₈ with corresponding percentage deviation with experimental values

V/V ₀	P (1)	$\Delta P(1)$ % div.	P(2)	$\Delta P(2)$ % div.	P(3)	$\Delta P(3)$ % div.	P(4)	$\Delta P(4)$ % div.	P(5)	$\Delta P(5)$ % div.	P(exp)
1.000	0.00		0.00		0.00		0.00		0.00		0.00
0.999	0.06	0.00	0.06	0.00	0.06	0.00	0.06	0.00	0.06	0.00	0.06
0.998	0.12	0.00	0.12	0.00	0.12	0.00	0.12	0.00	0.12	0.00	0.12
0.997	0.18	0.00	0.18	0.00	0.18	0.00	0.18	0.00	0.18	0.00	0.18
0.996	0.25	0.00	0.25	0.00	0.25	0.00	0.25	0.00	0.25	0.00	0.25
0.995	0.31	0.00	0.31	0.00	0.31	0.00	0.31	0.00	0.31	0.00	0.31
0.990	0.63	0.00	0.63	0.00	0.63	0.00	0.63	0.00	0.63	0.00	0.63
0.985	0.96	0.00	0.96	0.00	0.95	1.04	0.96	0.00	0.96	0.00	0.96
0.980	1.30	0.00	1.30	0.00	1.28	1.54	1.30	0.00	1.30	0.00	1.30
0.970	2.00	0.00	2.01	0.50	1.97	1.50	2.01	0.50	2.01	0.50	2.00
0.960	2.75	1.08	2.77	0.36	2.70	2.88	2.77	0.36	2.76	0.72	2.78
0.950	3.54	1.39	3.57	0.56	3.47	3.34	3.57	0.56	3.57	0.56	3.59
0.940	4.36	1.13	4.43	0.45	4.27	3.17	4.43	0.45	4.42	0.23	4.41

 Table – 6: Comparison of Variation of pressure P (in GPa) versus unit cell volume ratio (V/V₀) calculated by (1) Third degree Eulerian EOS (2) Third degree Lagrangian EOS (3) Second order B-M EOS (4) Third order B-M EOS (5) Bardeen EOS with experimental value for Nd_{1,32}Sr_{0,41}Ce_{0,27}CuO_{3.96} with corresponding percentage deviation with

	experimental values										
V/V ₀	P (1)	$\Delta P(1) \%$ div.	P(2)	$\Delta P(2)$ % div.	P(3)	$\Delta P(3)$ % div.	P(4)	$\Delta P(4)$ % div.	P(5)	$\Delta P(5)$ % div.	P(exp)
1.000	0.00		0.00		0.00		0.00		0.00		0.14
0.999	0.14	0.00	0.14	0.00	0.14	0.00	0.14	0.00	0.14	0.00	0.29
0.998	0.29	0.00	0.29	0.00	0.29	0.00	0.29	0.00	0.29	0.00	0.43
0.997	0.43	0.00	0.43	0.00	0.43	0.00	0.43	0.00	0.43	0.00	0.57
0.996	0.58	1.75	0.58	1.75	0.58	1.75	0.58	1.75	0.58	1.75	0.72
0.995	0.73	1.39	0.73	1.39	0.72	0.00	0.73	1.39	0.73	1.39	0.14
0.990	1.47		1.48		1.47		1.48		1.48		
0.985	2.25		2.25		2.23		2.25		2.25		
0.980	3.04		3.04		3.01		3.04		3.04		
0.970	4.70		4.71		4.63		4.71		4.71		
0.960	6.45		6.49		6.33		6.49		6.48		
0.950	8.29		8.38		8.13		8.38		8.37		
0.940	10.24		10.39		10.01		10.39		10.37		