Theoretical Prediction of Elastic Properties of Active and Smart Material at High Pressure

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Abstract: - This paper uses three different equations of states (I) Brennan - Stacey EOS, (II) Birch - Murnaghan EOS, and (III) Vinet - Rydberg EOS to theoretically predict the behavior of elastic properties of active and smart materials at high pressure under different compression, such as isothermal bulk modulus at different compressions, pressure derivative of isothermal bulk modulus, and Gruneisen parameter for CuO smart material. The outcome demonstrates that Gruneisen Parameter falls as compression rises. Additionally, when compression rises, the first derivative of isothermal bulk modulus drops.

Key Words: — ***Equation of state (EOSs), Smart Materials, Isothermal Bulk modulus, Gruneisen parameter.***

I. INTRODUCTION

Smart materials, also known as intelligent materials or responsive materials, are a class of substances that respond to environmental stimuli by behaving in a dynamic and adaptable way. These materials have drawn a great deal of interest from scientists, engineers, and researchers because of their outstanding qualities and possible uses in a variety of fields. When subjected to particular variables like temperature, stress, light, humidity, pH, or electric/magnetic fields, smart materials have the capacity to purposefully change their properties.

The idea of "smart materials" has its roots in antiquity, when natural materials like shape-memory alloys were used for a variety of purposes. But throughout the 20th century, substantial developments in material science and engineering opened the door to the creation of increasingly sophisticated and specialized smart materials.

This page provides a thorough review of smart materials, including all of their many varieties, basic operating principles, and potential applications.

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It also explores potential future developments and the difficulties involved in putting smart materials into commercial goods [1]

For these materials, the terms "smart" and "intelligent" are used reciprocally. Takagi described intelligent material are those that adapt to various environmental changes in the most efficient way possible [2].

Smart materials are advanced materials that can detect certain signals from the outside world and actuate themselves to do a specific activity. Smart, Intelligent, or even adaptive are words that come to mind [3-5]

II. METHOD OF ANALYSIS

In the current experiment we have used three different EOSs to study the thermo elastic property of smart materials.

- *Brennan*- Stacey EOS derived using thermodynamic formulation for Grüneisen parameter [6-7]
- *Birch* – Murnaghan (3rd-order) EOS derived using finite strain theory Brennan- Stacey EOS derived using thermodynamic formulation for Grüneisen parameter [8]
- *Vinet*-Rydberg EOS based on the universal relationship between binding energy and inter atomic separation for solids [9-10]

These EOSs are given below.

$$P = \frac{3B_0 x^{-4}}{(3B_0'-5)}\left[exp\left\{\frac{(3B_0'-5)(1-x^3)}{3}\right\} - 1\right] \quad (1)$$

$$P = \frac{3}{2}B_0[x^{-7} - x^{-5}]\left[1 + \frac{3}{4}(B_0' - 4)(x^{-2} - 4)\right] \quad (2)$$

$$P = 3B_0x^{-2}(1 - x)exp[\eta(1 - x)] \quad (3)$$

Where $x = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and $\eta = \frac{3}{2}(B_0' - 1)$.

Equation (1) is Brennan Stacey EOS, equation (2) is Birch Murnaghan (3rd-order) EOS and EOS of Vinet-Rydberg is equation (3). Where B_0 is the isothermal bulk modulus at zero pressure and B'_0 first pressure derivative of the isothermal bulk modulus at zero pressure, V is the volume at pressure P and V0 is the volume at zero pressure. Equation of state theory states that there is a correlation between the two parameters [11]

The formula provided by Borton and Stacey can be used to determine the value of the Grüneisen parameter (γ)[12]

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

Where f = 2.3

III. Result and Discussion

In this paper, we describe three different equations of state (EOS) for calculating pressure, isothermal bulk modulus (KT), first pressure derivative of isothermal bulk modulus (KT'), and gruneisen parameter at various compressions using equations (1-4). These EOS are Brennan Stacey EOS, Vinet Rydberg EOS, and Birch-Murnaghan EOS. The findings of the current study will be compared to those of recent investigations.

Table.1. Values of input data for B_0 (Gpa) and B_0' (Gpa)

Material	B_0	B_0'	References
CuO	81.00	4.0	[13]

Now Plotting a graph between Compression (V/V_0) and Pressure for smart material (CuO)

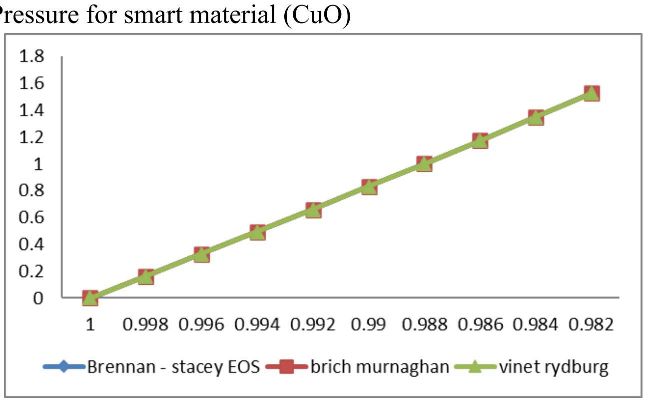

Fig.1. Pressure (P) Vs V/V_0 for CuO

Fig.1 it can be seen that that the three EOS give same result for the smart material used by us. These figures barely show any deviation while increase in pressure. The Three EOS shows similar value for pressure for the exact volume and also in the three EOS (Brennan-Stacey, Birch Murnaghan EOS and Vinet Rydburg EOS) for material CuO the value pressure shows continuous increment with decrease in contraction.

Now Plotting a graph between Compression(V/V_0) and Bulk modulus (K_T) for smart material (CuO).

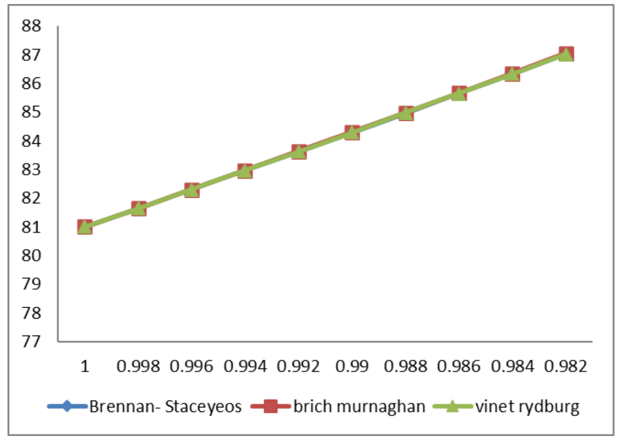

Fig.2. K_T Vs V/V_0 for CuO

Fig.2 shows the graph plotted between the isothermal bulk (K_T) modulus and V/V_0 and observes that K_T shows increment continuously with decrement in the volume in the three EOS (Brennan-Stacey, Birch Murnaghan EOS, Vinet Rydburg EOS) for the smart material CuO.

Now Plotting a graph between Compression(V/V_0) and First derivativeof Bulk modulus (K_T) for smart material (CuO).

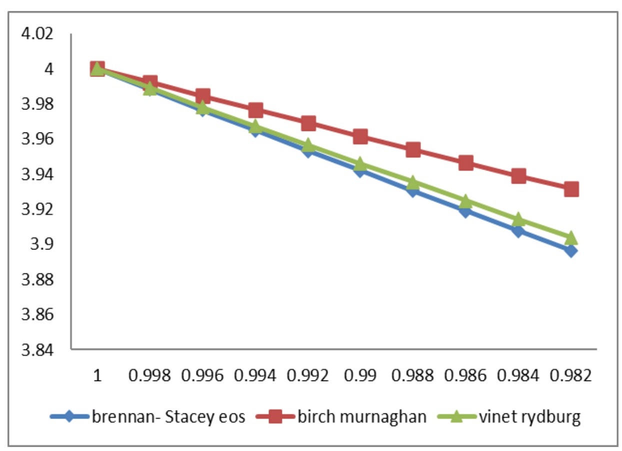

Fig.3. First pressure derivative of K_T Vs V/V_0 CuO

Fig.3 shows the graph between the first derivative of isothermal bulk (K'_T) modulus on the Y- axis and V/V_0 on the horizontal axis. We noticed that at point (3.989) all the EOS (Brennan-Stacey, Birch Murnaghan EOS, Vinet Rydburg EOS) are in the same phase for the smart material CuO. But after that the Birch Murnaghan EOS starts deviating with the other two EOS (Brennan-Stacey, Vinet Rydburg EOS). But after the point (3.956) two EOS (Brennan-Stacey, Vinet Rydburg EOS) starts deviating from each other.

Now Plotting a graph between Compression(V/V_0) and Grunesien parameter γ for smart material (CuO).

Fig.4 shows the graph presented between the Grunesien parameter in the y- axis and v/v_0 on the x- axis. we observed that Birch Murnaghan Eos start deviating from the origin from the other than EOS (Brennan-Stacey, Vinet Rydburg EOS) for smart material CuO. But after a point (1.0457) the other two EOS (Brennan-Stacey, VinetRydburg EOS) starts deviating from each other.

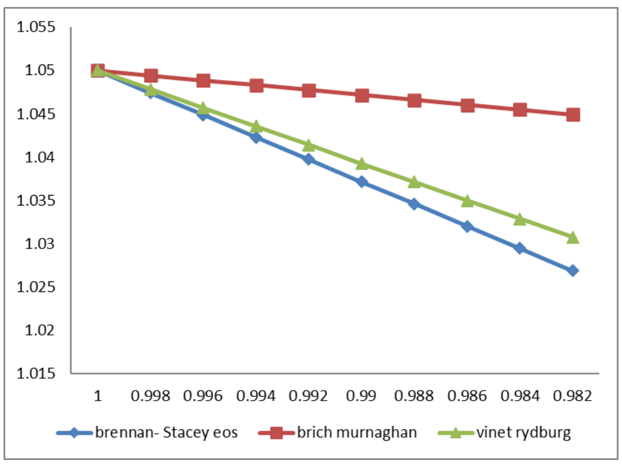

Fig.4. GrÜneisen parameter vs. $V/V_0$for CuO.

IV. Conclusion

The study investigated the equation of state (EOS) behavior of CuO smart materials using three forms. The results showed similar results with minimal deviation as pressure increased. The isothermal bulk modulus (KT) showed continuous increment with decreasing volume for all three EOS forms. However, at certain points, the Birch-Murnaghan EOS deviated from the other two forms. These findings can help understand material properties and behavior under different pressures and volumes.

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