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Theoretical Study of Mechanical, Elastic and Phonon Frequency Spectrum Properties for GaAs at High Pressure

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The calculations for variations of bulk modulus (B), compression volume $\left(\frac{V_p}{V_o}\right)$, lattice constant and phonon frequency spectrum (pfs) under high pressure up to 17 *GPa at room temperature has been carried out. Three equations of state (EOSs) including (Birch- Murnaghan, Vinet and modified Lennard-Jouns) are used in the calculations. The variations of these properties under such high pressure for GaAs are obtained and we got suitable EOS for it.*

Keywords: equation of state, Bulk modulus, compression, lattice parameter, phonon frequency spectrum.
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Introduction

The evaluation of pressure-volume (P-V) phonon frequency spectrum and lattice constant are very importance in basic and applied science (Recio et al. [12]), EOSs are fundamentally important in study the properties of solid state at high pressure, where the study of (P-V) EOSs of relevant material is one of the most basics are needed for pressure calibration. The Vinet, Birch–Murnaghan (BM) and modified Lennard–Jouns (mL-J) EOSs are intended to accounting volumetric properties for solid which has structural configurations that vary with pressure and temperature (Anderson [1]), BM EOS was derived from the assumption that the strain energy of a solid undergoing compression can be expressed as a Taylor series in the finite strain. (Birch [3]). The (mL-J) EOS was derived from interatomic potential (Jiuxun [6]) but Vinet EOS from relationship between variables (P, V) (Tripathi et. al. [15]). Phonon frequency spectrum curves for most solids shifts up slightly to the higher frequency values (Cüler & Cüler [8]).

In present work, the effect of pressure on bulk modulus (B), compression volume $\left(\frac{V_p}{V_o}\right)$, lattice constant and phonon frequency spectrum (PFS) for GaAs has been achieve using different EOSs.

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1. Theoretical Details

1.1. Equations of State (EOSs)

Birch–Murnaghan EOS. Suggested EOS for solids (Birch [2]) is given as:

$$P_{B-M}(V) = \frac{3}{2}B_o\left[\left(\frac{V_o}{V_\rho}\right)^{7/3} - \left(\frac{V_o}{V_\rho}\right)^{5/3}\right]\left\{1-\left(\frac{3}{4}\right)(4-B'_o)\left[\left(\frac{V_o}{V_\rho}\right)^{2/3}-1\right]\right\}, \quad (1)$$

where
Bo — thermal bulk modulus at atmosphere pressure,
B'_o — pressure bulk modulus derivative,
Vo — volume at atmospheric pressure,
Vp — volume at pressure P.

Vinet EOS. This EOS describe the relationship between the variables (P, V) and it was derived from a general inter-atomic potential (Grüneisen [5]). (Vinet el al. [16]) give suitable EOS as:

$$\rho_{Vinet} = 3B_o\left[\left(\frac{V_\rho}{V_o}\right)^{-2/3}\left\{1-\left(\frac{V_\rho}{V_o}\right)^{1/3}\right\}\right]\exp\left[\left(\frac{3}{2}\right)(B'-1)\left\{1-\left(\frac{V_\rho}{V_o}\right)^{1/3}\right\}\right]. \quad (2)$$

Modified Lennard–Jones EOS. (mL-J EOS) (Jiuxun [6])

$$P_{mL-J} = \frac{B_o}{n}\left(\frac{V_o}{V_P}\right)^n\left[\left(\frac{V_o}{V_P}\right)^n - 1\right], \quad (3)$$

where $n = \frac{1}{3}B'_o$; $B'_o = \frac{dB}{dp}$.

1.2. Bulk modulus

In general, bulk modulus given by

$$B = -V\left(\frac{dP}{dV}\right)_T \quad (4)$$

from derivation of Eqs. (1), (2) and (3) with respect to volume and substiting in Eq. (4) we get the bulk modulus equation as function of pressure which are given as:

$$B_{B-M} = \frac{3B_o}{2}\left[\left(\frac{7}{3}\right)\eta^{-7/3} - \frac{5}{3}\eta^{-5/3} - \frac{9}{4}\left(B'_o-4\right)\eta^{-3} + \frac{7}{2}\left(B'_o-4\right)\eta^{-7/3} + \frac{5}{4}(B'-4)\,\eta^{-5/3}\right], \quad (5)$$

$$B_{Vinet} = \left[2B_o\left(\eta^{-2/3} - \eta^{-1/3}\right) + B_o\eta^{-1/3} + \frac{3}{2}B_o\left(B'_o-1\right)\left(\eta^{-1/3}-1\right)\right]\times \times e^{\left[\left\{\frac{3}{2}\left(B'_o-1\right)\right\}\left(1-\eta^{1/3}\right)\right]}, \quad (6)$$

$$B_{mL-J} = B_o\left(\frac{V_o}{V}\right)^n\left[2\left(\frac{V_o}{V}\right)^n - 1\right]. \quad (7)$$

1.3. Lattice constant

Radi et al. [11] determined the variation of lattice constant with the pressure according to Murnaghan EOS (Murnaghan [10]).

$$a_p = a_o \left(1 + B_o^{'} \frac{P}{B_o}\right)^{-\frac{1}{3B_o^{'}}}, \tag{8}$$

where a_o is Lattice parameter at atmosphere pressure, a_p is Lattice parameter at pressure P.

From Murnaghan EOS

$$\frac{V_p}{V_o} = \left(1 + B_o^{'} \frac{P}{B_o}\right)^{-\frac{1}{B_o^{'}}}. \tag{9}$$

Then Eq. (8) can be written as:

$$a_p = a_o \left(\frac{V_p}{V_o}\right)^{-\frac{1}{3}}. \tag{10}$$

1.4. Phonon frequency spectrum (PFS)

The pressure applied on the solid causes many changes in the internal atomic forces. Therefore, the properties of the solid under high pressure can vary (Dlouha [4]). In this study, the effect of pressure on the lattice constant and the density of state for GaAs calculated by using Grьneisen approximation to calculate the variation of the frequency where variation of mode density due to the specific volumes change of the crystal using the above equations of state (1), (2) and (3).

2. Calculations and Results

2.1. Calculations of compression volume $\left(\frac{V_p}{V_o}\right)$ for GaAs under high pressure.

On substituting the values B_o, B_o' tabulated in Tab. 1 in to Eqs. (1), (2) and (3).

Table 1. Values of bulk modulus (B_o), its derivative (B_o') and lattice constant a_o for GaAs

B_o	74.7GPa	(Hanfland, et al. [9])
B_o'	4.67	(Hanfland, et al. [9])
a_o	5.650$\dot{A}$	(Levenshtein and Rumyantsev [7])

Obtained results for $\left(\frac{V_p}{V_o}\right)$ variations under high pressures are shown in Fig. 1, in comparison with experimental data published in the scientific literatures.

2.2. Calculations of variations bulk modulus B_o with high pressure for GaAs using B.M, Vinet, and mL.J EOSs

On substituting the values of B_o, B_o' tabulated in Table (I), into Eqs. (5), (6) and (7). Obtained results for variations of bulk modules, for GaAs, are showing Fig. 2 with high-pressure give us the values of bulk modulus according to the values of $\left(\frac{V_p}{V_o}\right)$ at different values of pressure by using different EOS (Fig. 2).

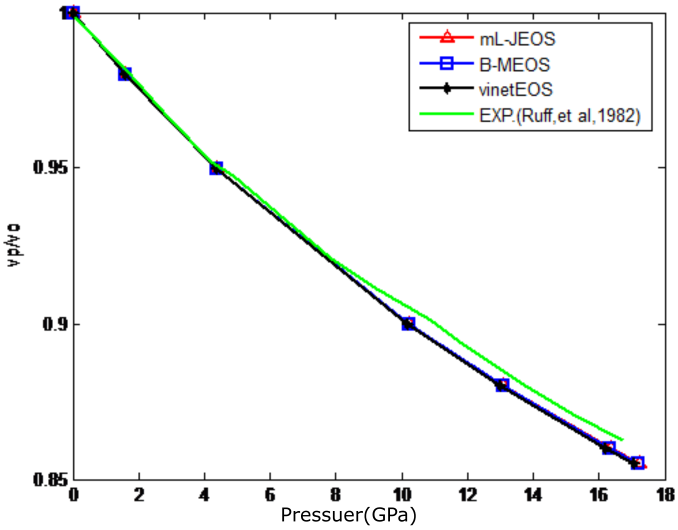

Fig. 1. Variation of $\left(\frac{V_p}{V_o}\right)$ for GaAs at different values of pressure, using BM, Vinet, mL.J EOSs comparison with other experiment data

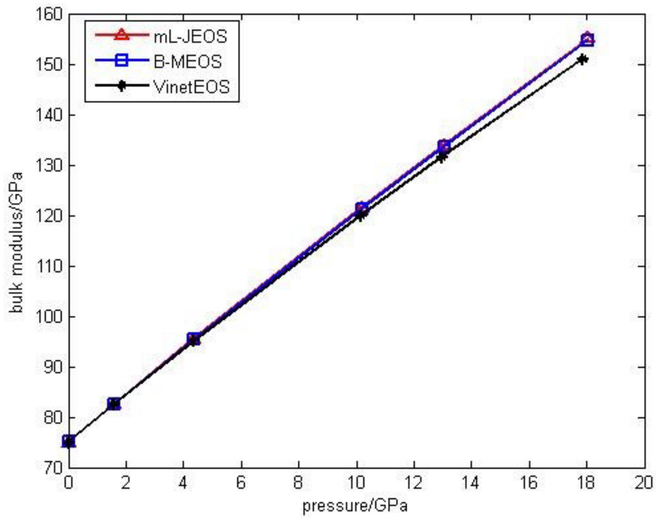

Fig. 2. Variation of bulk modulus B_o for GaAs at different values of pressure, using BM, Vinet & mL-J EOSs

2.3. Calculations of lattice constant variations, for GaAs, under high pressure

On using Eq.(10) with ($a_o = 5.650\dot{A}$, for $GaAs$) (Levenshtein and Rumyantsev [7]), and $\left(\frac{V_p}{V_o}\right)$ data from Fig.1. Present result for variations of lattice constant, for GaAs, with pressure are shown in Fig. 3. on comparison with experimenter data of (Ruoff et al. [14]).

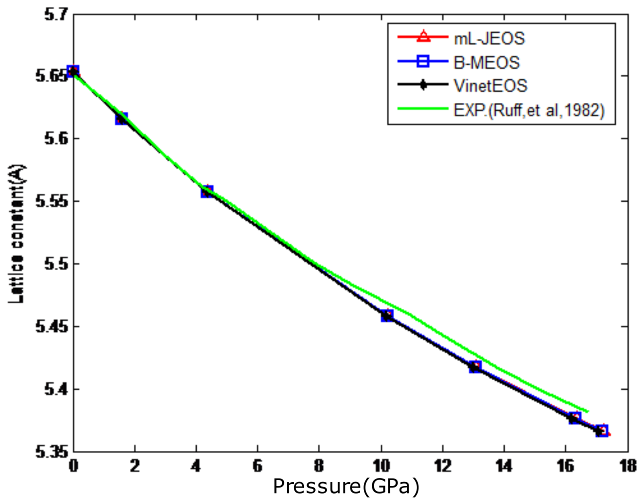

Fig. 3. Variation of lattice parameter for GaAs with high pressure using different EOSs

2.4. Evaluations of (PFS), for GaAs, under high pressure using (BM, Vinet, mL.J) EOSs

Fig. 4 shows phonon frequency spectrum for GaAs at atmospheric pressure and room temperature

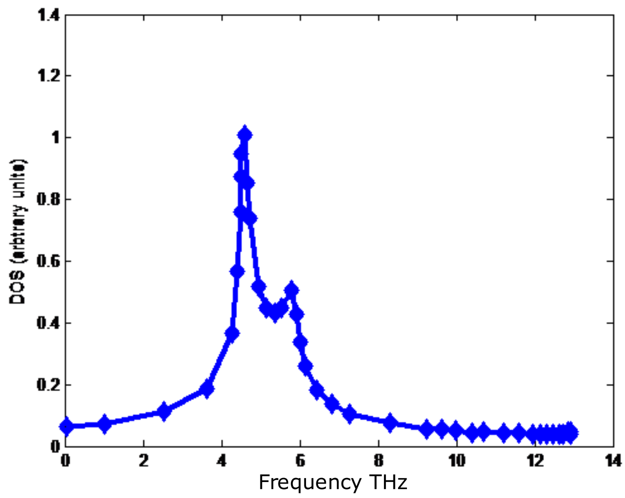

Fig. 4. Variation of frequencies of GaAs at atmosphere pressure (Fu & Maguchi [17])

Since any change in $\left(\frac{V_p}{V_o}\right)$ produce, a change in the equilibrium position of lattice point and it will produce a change in the frequency spectrum, which is given as (Dlouha [4]):

$$\upsilon_p = \upsilon_o \left(\frac{V_p}{V}\right)^{-\gamma}, \tag{11}$$

γ: Grneisen parameter at atmosphere pressure

$$g(\upsilon, V_p) = \left(\frac{V_p}{V}\right)^{\gamma} g[\upsilon_o, V_o], \tag{12}$$

υ_o — frequency at atmospheric pressure,
υ_p — frequency at pressure P.
From Eqs. (11) and (12), and putting $\gamma = 1.73$, for GaAs, (Resul and Irving [13]), and using $\left(\frac{V_p}{V_o}\right)$ shown in Fig. 1. Obtained results for variation of GaAs phonon frequency spectrum under high pressure by using different equation of state are shown in Figs. 5–7.

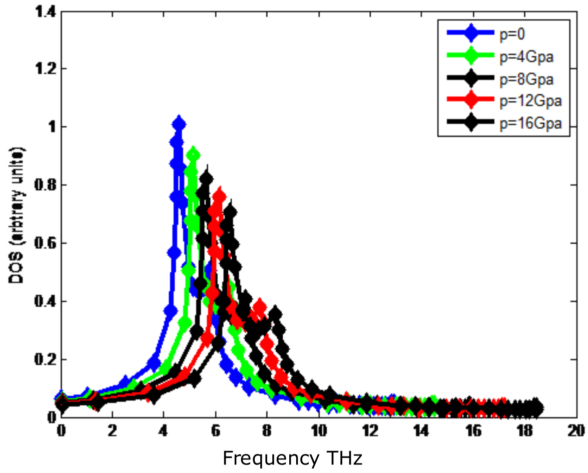

Fig. 5. Variation of frequencies with pressure for GaAs using Birch-Murnaghan EOS

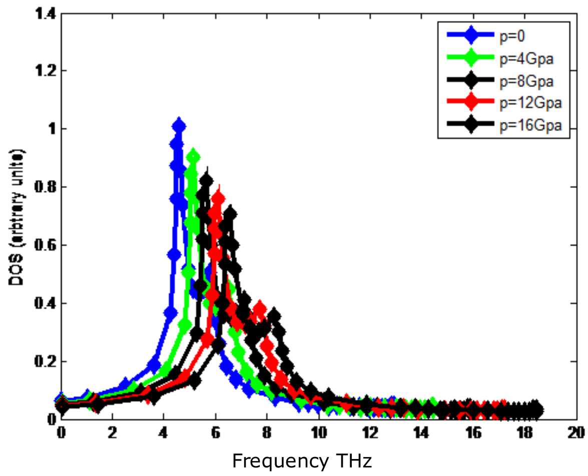

Fig. 6. Variation of frequencies with pressure for GaAs using mL.J EOS

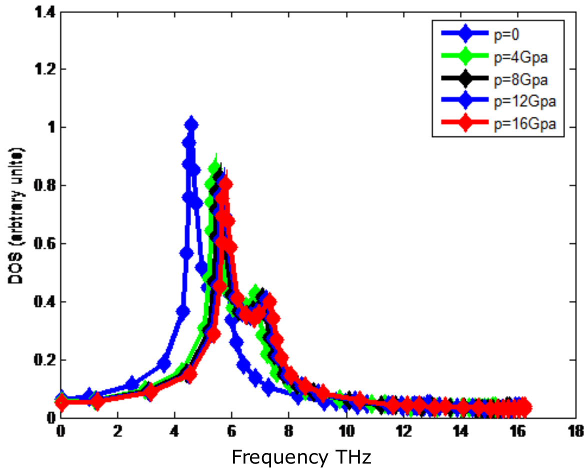

Fig. 7. Variation of frequencies with pressure for GaAs using Vinet EOS

3. Discussion and Conclusion

Variations under high pressure of $\left(\frac{V_p}{V_o}\right)$, Bulk modulus, lattice constant for GaAs have been evaluated by using three different EOSs given in Eqs. (1), (2) and (3). All the three different equations give an excellent agreement between their results in comparison with experimenter data. On evaluating variations of (pfs) for GaAs under high pressure B.M EOS (Eq. (1)) and mL-J EOS (Eq. (3)) give a reasonable shift to higher frequencies in agreement with theoretical interpretation for the effect of high pressure on pfs for solids. While Vinet EOS (Eq. (2)) cannot give a coincidence results with B.M and mL-J EOSs results.

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Теоретическое исследование механических, упругих и фононных частотных свойств GaAs при высоком давлении

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Представлены расчеты для изменения объемного модуля (B), объем сжатия $\left(\frac{V_p}{V_o}\right)$, *постоянная решетки и спектр фононных частот при высоком давлении до 17 ГПа при комнатной температуре. В расчетах используются три уравнения состояния EOS, в том числе Берч-Мурнаган, Винет и модифицированный Леннард-Джунс. Получены вариации этих свойств при высоком давлении для GaAs и подходящие EOS для них.*

Ключевые слова: уравнение состояния, объемный модуль, сжатие, параметр решетки, спектр фононных частот.