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Comparative Study of Phonon Density of State for Platinum under High Pressure: Grüneisen Approximation Approach

Adnan M. Al-Sheikh, Hamsa B. Al-Bazaz and Raed Hashim AL-Saqa
Dept. of Physics, Collage of Science, University of Mosul, Iraq
Dept. of Environmental Technologies, Environmental College University of Mosul, Iraq
Tatwaan Secondary School Directorate General of Education, Province of Nineveh, Iraq

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Abstract:
The phonon density of state (PDOS) for platinum was studied under high pressures and different volume compression by using Grünesien approach and different equations of state (EOSs), Birch-Murnaghan EOS and Bardeen (EOS),Birch-Murnaghan EOS which is based on the solid mechanics definition of finite strain and Bardeen (EOS) which basedon inters atomic potentials. The obtained results are compared with the results of Abinitio calculations. This work reveals the importance of considering Grünesien parameter variation under high pressure to shows how to get rid of difficulties in evaluating (PDOS) using EOS for solids

Keywords: *phonon density of state, Grüneisen approach, equation of state, high pressure, Platinum..*

I. INTRODUCTION

When solids exposed to high pressure, several effects take place, first the symmetry of the crystal changes by strain generated within the crystal by applied pressure this leads to Phonons modes density mixing and thus inactive phonons modes density become active, second, Lattice frequency is often shifting to higher frequencies as a result of volume compression and third Intensities of vibrational band can changed as a result of pressure induced dipolemoment and changing in polarizability[1].
Platinum (Pt) is a heavy element and has an electronic arrangement [Xe] $4f^{14}5d^{9}6s^{1}$.The [Xe] states core states while the other states considered as valence state [2]. There is a difference between 3d and 5d transition elements, since the 5d orbit is more remote than 3d orbit, which made its coulomb interaction somewhat weaker [3].

The stable state of Platinum at ambient pressure is face-center-cubic (FCC) and it is stable to very high pressure, about 650 GPa[4] due to this stability Platinum is therefore widely used in the calibration of P-TX-ray diffraction measurements [5-6].

This work present a Grüneisen approximation approach using different equations of state (EOS's) to evaluate phonon density of states (PDOS) for Platinum under high pressure in comparison with abinitio first principle calculations(AFPC) of[4].

II. THEORETICAL DETAILS

Since the phonon density of state (PDOS) spectrum related to the thermodynamic instability, so we can use the equation of state (which consider the most fundamental thermodynamic quantities P-V-T to understand the behavior of materials under high pressure and high temperatures) to show the PDOS behavior at different pressures. The lattice frequencies under high pressure shift to higher frequencies, while the mode density spread to give new modes [7]

Grünesien approximation:

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To study phonon frequency spectrum under high pressure it is useful to explain that any change in the specific volume Vo of a crystal causes a change in the equilibrium positions of the lattice points and thus a change in the phonon frequency spectrum. Even, only isotropic volume changes are considered, frequencies of the vibrations will change as functions of the changes of at least two elastic constants, each of which will generally have a different dependence on the specific volume, this cause a change in specific volume of the crystal is reflected in a change of its frequency spectrum in a very complex manner. To overcome The difficulties of calculating phonon frequency spectrum for different volumes at the least approximately, Grüneisen approximation expressed the connection between ν_o and ν_p of corresponding frequencies at specific volume Vo and Vp respectively in the following relations [8].

$$\nu p=\nu o(V/Vo)^{-\gamma_o} \quad \ldots\ldots(1)$$

While the change in the density of stateis expressed by the relation:

$$gp= (\nu p , Vp)=(V /V_o)^{\gamma o} g(\nu_o,V_o)$$

Where:

$\nu_p$frequency at pressure (P).

ν_o:Frequency at atmospheric pressure.

γ_o:Grüneisen parameter at atmospheric pressure

$g_p(\nu_p,\nu_p)$:Phonon density of state at pressure (p).

$g(\nu_o,V_o)$:Phonon density of state at atmospheric pressure.

V:volume at pressure(P)

V_o: volume at atmosphericpressure.

Equations of state(EOSs):

EOSs are fundamentally important in the study of the properties of a solid state under high pressure, where the study of (Volume-Pressure) EOSs of relevant materials is one of the most basics are needed for pressure calibration [9].

The EOSs which are used in this work are Birch-Murnaghan and Barden EOS's,

Birch-Murnaghan (B-M) EOS, which is based on the solid mechanics definition of finitestrain and has the form Birch [10-11]

$$P_{B-M}(V)=\frac{3k_o}{2}\left[\eta^{-7/3}-\eta^{-5/3}\right]\left[1+\frac{3}{4}(k'_o-4)\left(\eta^{-2/3}-1\right)\right] \quad (3)$$

Barden (B) EOS which based on interatomic potentials and has the form[12]:

$$P_B(V)=3k_o\left[\eta^{-5/3}-\eta^{-4/3}\right]\left[1+\frac{3}{2}(k'_o-3)\left(\eta^{-1/3}-1\right)\right] \quad (4)$$

Where:$k_o, k_o'$are the Bulk modulus and its first pressure derivative respectively, and η=V/V_o

Table I Shows values of different parameters for Platinum (Pt).

TableI: Values of Bulk modulusk_o,Bulk modulus first derivative$k_o'$and Grüneisen parameter all at atmospheric pressure for Platinum.

Parameter	Value
k_o	278 GPa ref. [13]
k_o'	5.61 ref. [14]
γ_o	2.56 ref. [15]

III. GRÜNEISEN PARAMETER

The Grüneisen parameter has both macroscopic and microscopic definitions. The macroscopic definition is in terms of thermodynamic quantities given as [16]

$$\gamma_o=\frac{\alpha_V K_o}{C_V \rho} \quad (5)$$

Where α_v: volume coefficient of thermal expansion

ρ: density.

C_V: specific heat at constant volume.

The microscopic definition arises from vibration of atoms in a solid, as the vibrational frequencies of the individual atom in a solid varied with volume V, via the relation

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$$\gamma_o = \frac{\partial \ln \nu}{\partial V} \quad (6)$$

Where,ν is frequency of vibration.

A relation for pressure (volume) dependence of Grüneisen parameter is given in [17]

$$\gamma_p = \gamma_o(\eta)^q \quad \ldots\ldots\ldots\ldots\ldots\ldots (7)$$

Where γ_p is Grüneisen parameter at high pressure P, and q: is 2nd Grüneisen parameter, (q=0.5 for Pt) [2].

IV. Calculations andresults

Compression volume

on using the two different EOSs (Birch- Murnaghan and Bardeen) given in equations 3 and 4, respectively, different high pressure values and their corresponding V/V0 values have been computed and tabulated in Table II

Table II: Compression volume,η=V/V_oversus Pressure, P, for Platinum, Pt as using B-M EOS Equ. (3) and B EOS Equ (4)

	Pressure values (GPa)	
η	***B-M EOS***	***B EOS***
1.0000	0	0
0.9500	16.4645	16.4399
0.9000	39.3461	39.1077
0.8687	58.0555	57.4442
0.8500	71.2088	70.2261
0.8000	115.8077	112.9295
0.7500	178.7482	171.7116
0.7430	189.4382	181.5427
0.7000	268.5815	253.1351
0.6711	337.7281	314.1781
0.6500	398.6804	366.9916

Fig.1: shows variation of η with P, for platinum evaluated by using B-M and B EOSs, equations (3) and (4), respectively.

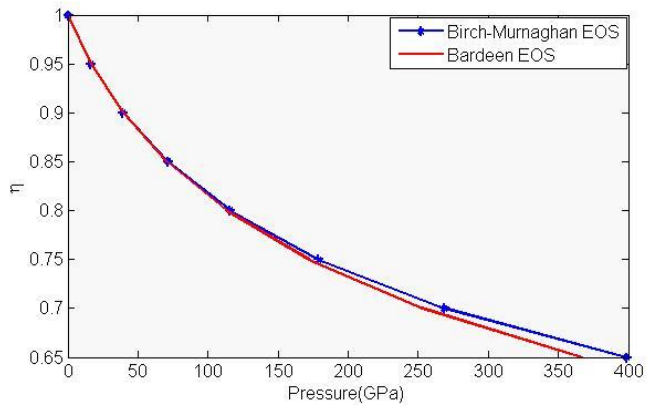

Fig.1: Compression volume η versus pressure using B-M and B EOSs

PDOS under high pressure

Fig.2: shows PDOS for platinum at atmospheric pressure.

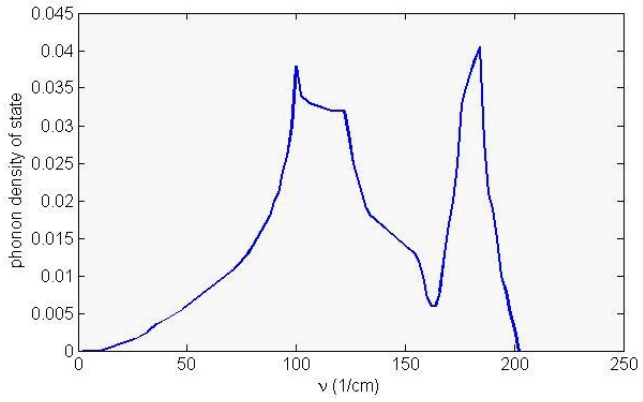

Fig. 2: The phonon density of state for Platinum at atmospheric pressure
[4].

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On analyzing phonon frequency spectrum (pfs) of Fig. 2 and substituting η values of Table II into equations (1) and (2), Fig. 3 shows platinum pfs under high pressure evaluated by using B-M and B EOSs and Grüneisen approximation in comparison with *abinitio* high pressure results of [4].

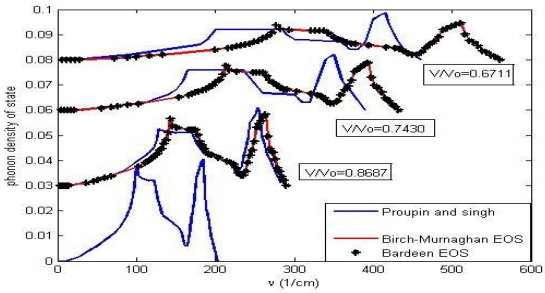

Fig.3: Platinum PDOS under 12 high pressure, with Grüneisen parameter(γ_o) be volume independent, comparison with *abinitio* calculations [4]

Although the present results, shown in Fig.3, by using (B-M and B) EOSs are ingood agreement with each other, but still both of them are in poor agreement with results obtained by *abinitio* calculations of [4]

Volume dependence of γo parameter

On considering variation of γo parameter with high pressure, as given in equation (7),
equations (1) and (2) modified to the forms of equations (8) and (9) respectively

$$v_{p\gamma} = v_o \left(\frac{V}{V_o}\right)^{-\gamma_p} \qquad (8)$$

$$g_{p\gamma}(v_p, V_p) = \left(\frac{V}{V_o}\right)^{\gamma_p} g(v_o, V_o) \qquad (9)$$

By repeating the calculations of the effect of high pressure on PDOS of platinumas showed inFig.1using equations (8) and (9) and Table-II data. The results shown in Fig.4represents the pfs calculations for platinum were obtained using B-Mand BEOSs, after taking into account variation of γ_o under high pressure, in comparison with *abinitio* calculations Proupin and Singh [4]

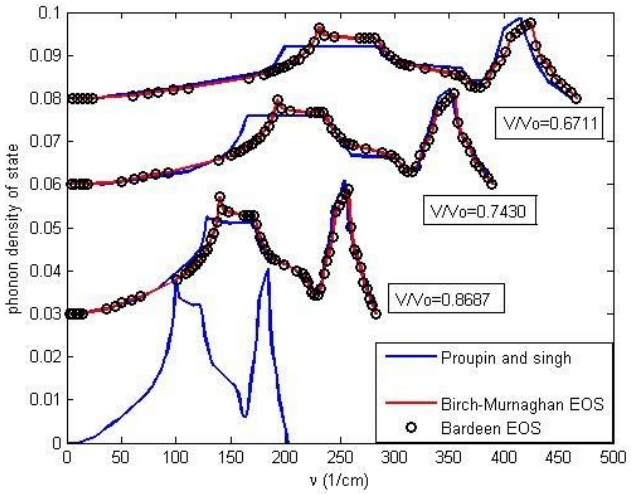

Fig.4: Platinum PDOS under high pressure evaluated using B-M and B EOSs considering variations of $\gamma_o$under high pressure in comparison with [4] calculations.

V. Discussion and Conclusions

Fig. 3 and Fig. 4 show phonon modes are shifted to a higher energies as high pressure increases, this may be attributed to the fact that the external pressure compresses the inter atomic distance causing stiffer bonds. Despite B-M EOS based on mechanical properties of solid and Bardeen EOS based on inter atomic potential, Fig. 3 shows results evaluated by using both EOSs are in a very good agreement with each other but they are in poor agreement with abinitio calculations of [4]. While Fig.4 shows an improvement in the present results, as a good agreement is achieved between present work and abinitio calculations of[4] this reveal the importance of considering pressure (volume) dependence of Grüneisen parameter (γo). Even though abinitio calculations has its own limitations related to basic material parameters and basic set, but in the present work depending on Grüneisen approximation shows well agreement with it.

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