

**Original Article** 

### Phonon Dispersion Relation of Lead (Pb) and Palladium (Pd)

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### ABSTRACT.

The Computational theoretical techniques were applied in the investigation of Phonon Dispersion of Lead (Pb) and Palladium (Pd). The first principle technique makes use of the density functional theory as implemented by quantum expresso as well as interatomic force constant (IFC) techniques (Born-von Jarman) which was extended to a higher number of neighbors than what is available in the literature were employed in this research. The results obtained show that the local density approximation (LDA) phonon dispersion slightly overestimates experimental results whereas the generalized gradient approximation (GGA) gives a slightly lower frequency. However, there was a negligible improvement in the quality of fit in the lead when the ninth neighbor (1 - 9NN) interaction was introduced.

Keywords: Phonon, Quantum expresso, Eigen – value, Lead(Pb), Palladium(Pd)

### **INTRODUCTION**

The physical properties of Lead(Pb) and Palladium(Pd) are of strong scientific interest – fundamentally as a highly correlated electronic system and technologically. Recent interest in hydrogen storage systems and nanoscale devices has highlighted the crucial role palladium plays in a wide range of systems. Hydrogen sensors based on Pd nanowires show both fast response and low power requirements. Recent experimental

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work indicates that Pd leads provide ohmic contacts for nanotube field effect transistors, a feature crucial for large scale device integration. In addition to nanoscale applications, bulk palladium also presents interesting properties that have fascinated researchers for years. It possesses a high magnetic susceptibility and sits on the edge of magnetism. Perhaps due to this, no measurable superconductivity has been found in the system for any temperature. Phonon scattering events play a crucial role in both superconductivities in bulk systems and transport in nanoscale interconnects. In this work, we examine the phonon dispersion of lead and palladium from a first principles perspective. Recent advances in density functional perturbation theory (DFPT) have made it possible to examine the acoustic properties of materials at a level of accuracy previously reserved only for electronic properties. Prior to the development of this approach, researchers were forced to use a frozen phonon technique that required large supercells or phenomenological approaches that relied on numerous fitting parameters (Stewart, 2008). Lead is still widely used for car batteries, pigments, ammunition (shot and bullets), cable sheathing, weights for lifting, weight belts for diving, lead crystal glass, radiation protection and as a constituent of solder, type metal, bearing alloys, fusible alloys, and pewter. Palladium on the other hand is widely used in catalytic reactions in industry, such as in hydrogenation of unsaturated hydrocarbons, as well as in jewelry and in dental fillings and crowns. But the main use of palladium, along with rhodium and platinum, is in the three-way catalytic converters in car exhaust systems.

The largest use of palladium today is in catalytic converters. Palladium is also used in jewelry, dentistry, watch making, blood sugar test strips, aircraft spark plugs, surgical instruments, and electrical contacts. Palladium is also used to make professional transverse (concert or classical) flutes. As a commodity, palladium bullion has ISO currency codes of XPD and 964. Palladium is one of only four metals to have such codes, the others being gold, silver and platinum. Because it adsorbs hydrogen, palladium is a key component of the controversial cold fusion experiments that began in 1989.

Solids, liquids and gases are made up of atoms which are in constant motion at all temperature even at absolute zero temperature (Kittel, 1996). The atoms in solids execute small oscillations with energy governed by the temperature of the solids. The small oscillations in crystals are known as lattice vibration; when atoms vibrate they emit phonons. Phonons are the packets of sound energy created by vibrations inside a material. Lattice dynamics originated in 1905, with Einstein's confirmation, via history of Brownian motion, that atoms exist (Einstein, 1905; Einstein, 1906), Within two years, Einstein had shown, using Planck's theory of radiation, that the temperature – dependence of the heat capacity of solids could be explain through the quantization of atomic vibrations (Einstein, 1907).

Phonon dispersion relation in crystals may be determined either experimentally or theoretically. Most experimental techniques determine the frequencies of lattice vibrations by inelastic neutron scattering experiments (Kazanc and Ozgen 2008) or by thermal diffuse x-ray scattering experiments (Burkel *et al*, 1987 and Dorner *et al*, 1987). Theoretical techniques focus on solving the Schrodinger wave equation (SWE) for a given lattice system and deriving the force constant (ie the second derivative of the total crystal potential energy with respect to atomic separation) of the system from which the phonon frequencies are calculated by generating and using the corresponding dynamical matrix. The dynamical matrix is the fourier transform of the force constant (Ruf *et al* 2001; Bencherif *et al*, 2011).

The theoretical approaches are divided into broad groups, namely, the empirical (or phenomenological) and the ab initio (or first principles methods). The empirical methods make use of adjustable parameters to fit experimental data to construct empirical models. On the other hand, ab initio methods have no need for empirical fitting parameters, but they generally employ a variational approach to calculate the ground-state energy of a many-body system from which the force constant and the associated dynamical matrix are obtained for use in computing the phonon frequencies (Baroni *et al*, 2001). The major shortcomings of the empirical approaches are that they are not necessarily applicable to all types of solids, and their parameters do not contain conceptual simplicity (Srivastava, 1990). On the other hand, the ab initio methods are only suitable for investigating systems in their ground-state configurations, thus unsuitable for investigating excited systems (Dreizler and Gross, 1990; Martin 2004).

These methods use technique different from that employed in phenomenological models to determine the total energy in the crystal. The DFT which is basically a many electron theory (Dreizler and Gross, 1990) pictures the potential energy in the crystal as a functional of the electrons density. Through the choice of a basic ground state parameter of the system, say the many-electron density, a self-consistent calculation of the Kohn-Sham potential (Martin, 2004) is carried out iteratively until convergence that is employed as the potential energy in the Schrodinger Wave Equation (SWE) which is then solved for the phonon frequencies.

The aim of this research is to obtain the phonon dispersions of two Face Centered Cubic (FCC) metals namely Lead (Pb) and Palladium(Pd) from accurately determined interatomic force constants (IFCs) using quantum expresso code, IFC approach up to at least sixth neighbour and compare phonons results with experimental data.

### THEORETICAL CALCULATION AND CONSIDERATIONS

### **Adiabatic Approximation**

The adiabatic (Born-Oppenheimer) approximation allows one to decouple the motion of the atom (core) from the motion of the valance electrons as though the nuclei were

fixed in their instantaneous positions (Slater, 1963 and Ziman, 1965). In a metal, the crystal is made up of ions and mobile valence electrons which interact with each other through Columbic forces. In other to construct the Hamiltonian for the ionic motion, which is the focus in the theory of lattice dynamics both the ionic coordinates and valence electron coordinates must be treated independently and this is made possible by the adiabatic approximation.

The adiabatic principle states that the eight-states of the valance electrons adjust themselves instantaneously to the position of the ions in the vibrating lattice (Born and Oppenheimer, 1927; Scrivastava, 1990). This is made possible as the nuclear mass is much larger than electron mass; and also the ions have energy level spacing which is much smaller than those of electronic states.

The Schrodinger equation for a system containing n electron and N nuclei can be represented as an Eigen value problem (Lin, 2005)

$$\mathrm{H}\psi(r_{i}--r_{n},R_{i}--R_{N})=\varepsilon\psi(r_{i}--r_{n},R_{i}--R_{N})$$
(2.1)

Where  $\psi$  is the wave function,  $\varepsilon$  is the total energy in the system,  $R_i$  are the  $i^{th}$  electron and ionic coordinates respectively

The Hamiltonian (H) in equation (2.1) can be written as

$$H = -\sum_{i} \frac{h^{2} \partial^{2}}{2m \partial r_{l}^{2}} - \sum \frac{h^{2} \partial^{2}}{2m \partial r_{i}^{2}} + \sum_{i>j} \frac{e^{2}}{\left|r_{i} - r_{j}\right|} + \sum V_{b}\left(r_{l} - R_{l'}\right) + \sum_{l,i} V_{b}\left(r_{i} - R_{l}\right)$$
(2.2)

Where  $R_i$  is the position of the  $i^{th}$  ion relative to the  $i^{th}$  site in a bravais lattice, and  $r_i$  represents the position of the  $i^{th}$  electron. Here, the summation is taken over all the ions and valence electrons in the system. The first two terms denotes the kinetic energy of the ions and the electrons of masses M and m respectively. The third term is the bare coulomb interaction between the electrons; and the fourth term is the pairwise bare ion-ion interaction. While the fifth term is the bare ion-electron interaction

$$r_{i-}r,$$
  
 $R_i-R,$ 

According to the adiabatic approximation we assume that the coordinates of the ions are instantaneously fixed. If  $\psi(\mathbf{r},\mathbf{R})$  is an eigen-function satisfying the Schrodinger equation for electrons then we may write:

$$\left\{-\sum \frac{h^2 \partial^2}{2m \partial r_i^2} + \sum_{i>j} \frac{e^2}{|r_i - r_j|} + \sum V_b(r_i - R_l)\right\} \psi_n(r, R) = \mathcal{E}_n(R) \psi_n(r, R)$$
(2.3)

 $E_n(R)$ , is the energy eigen – value of the electron which depends on the instantaneous ionic coordinates.

For the total Hamiltonian, we write the wave function as:

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$$\psi(r,R) = \psi_n(r,R)x(R) \tag{2.4}$$

If the ion Hamiltonian is

$$H_{i} = -\sum_{i} \frac{h^{2} \partial^{2}}{2m \partial r_{l}^{2}} + \sum_{i} V_{b} (r_{l} - R_{l'})$$
(2.5)

We then add  $E_n(R)$  to it and put the total wave function to solve the Schrödinger equation

$$H = \left\{-\sum_{i} \frac{h^2 \partial^2}{2m \partial r_i^2} + \sum W_b(r_i - R_{i'}) + \operatorname{E}(R)\right\} \psi_n(r, R) x(R) = \operatorname{E} \psi_n(r, R) x(R)$$
(2.6)

Where E is the total energy, evaluating the first part of equation (2.6) we obtain

$$\left\{-\sum_{l}\frac{h^{2}\partial^{2}}{2M\partial R_{l}^{2}}+\sum_{l>l'}W_{b}\left(R_{l}-R_{l'}\right)+\mathrm{E}_{n}\left(R\right)\right\}x(R)=Ex(R)$$
(2.7)

Equation (2.7) remains true if we make the assumption that the equation

$$-\sum \frac{h^2}{2M} \left\{ \frac{2\partial \psi_n(r,R)\partial x(R)}{\partial R_l^2} + x(R) \frac{\partial^2 \psi_n(r,R)}{\partial R_l^2} \right\}$$
(2.8)

May be neglected; since the first term of the equation (2.9) results in the integral of the form:

$$\int x_n^* \frac{\partial x_n}{\partial R_l} \partial r = \frac{1}{2} \frac{\partial}{\partial R_l} \int x^* x \, \partial r = \frac{1}{2} \frac{\partial n_e}{\partial R_l} = 0$$
(2.9)

Where  $n_e$  is the total number of electrons and  $\frac{\partial n_e}{\partial R_i} = 0$  is the rate of change with respect of electrons in the crystals. The second term of equations (2.9) is small for electrons tightly bound to the ions, so that  $\psi_n(r, R) = \psi(r_i - R_l)$ . Hence we obtain

$$-\int \psi_n^* \frac{h^2 \partial^2 \psi_n}{2M \partial R_l^2} \,\partial r = -\int \psi_n^* \frac{h^2 \partial^2 \psi_n}{2M \partial R_l^2} \,\partial r = -\frac{m}{M} \int \psi_n^* \frac{h^2 \partial^2 \psi_n}{2M \partial R_l^2} \,\partial r \tag{2.10}$$

Equation (2.10) is the product of  $\frac{m}{M}$  and the kinetic energy of the electron in its motion round the ion at  $R_l$ . This is small since  $\frac{m}{M} < 1840$  and of the order  $10^{-4}$  or  $10^{-5}$ 

From the derivations so far, the ionic and electron motions have been separated. The only electron-phonon interaction is the one due to transitions between electron states as the ions move.

# Calculation of The Phonon Dispersions of Pb and Pd with One Atom Per Unit Cell

The application of the Born-von karman theory (Born and Huang, 1954) to fcc lattices have been described by many authors. Pb and Pd belong to the space group of  $0_h^5$  (Fm 3m) with underlying point group  $O_h(m3m)$ . In calculating the phonon dispersions, we start by assigning inter atomic force constant matrix to the first atom of a particular neighbor. This is achieved using the coordinates of the neighbors of a particular atom. The interatomic force constant  $\phi_{\alpha\beta}$  is defined to be the force on the origin atom in the "  $\alpha$  direction when the atom moves a unit distance in the " $\beta$  direction. The force constant matrix  $\phi_{\alpha\beta}(0,l)$  is symmetric.  $l_1$ ,  $l_2$ ,  $l_3$  are three non- negative integers with  $l_1 \ge l_2 \ge l_3$ . We consider the metals: Pb and Pd as cubic crystals of identical atoms of mass (m) with cubic side of length (a) with coordinate axes along three tetrad axes x, y, z.

### **PRESENTATION OF RESULTS**

The results of the phonon dispersion for Pb are presented in section 3.1 while the results of the phonon dispersion relation for Pd from interatomic force constants (IFCs) approach and quantum espresso code are presented in section 3.2.

### **Phonon Dispersions of Lead(Pb)**



**Figure 3.1.1**: Calculated phonon dispersions for fcc-Pb compared to inelastic neutron scattering data (black circles) Dal corso (2008)



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Pb	a(a.u)	Хт	$\mathbf{X}_{\mathbf{L}}$	WT	$W_L$	LT	$\mathbf{L}_{\mathbf{L}}$
EXP (a)	9.27	0.90	1.80	1.47	1.71	0.90	2.19
LDA(b)	9.19	1.09	1.93	1.80	1.89	1.06	2.56
GGA(b)	9.51	1.16	1.71	1.47	1.73	0.97	1.98

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a Dal corso (2008)

b This work



**Figure 3.1.2:** Calculated phonon dispersions for fcc-Pb from analytical approach using IFCs up to 9<sup>th</sup> neighbour

<b>Table3.1.2</b> : Frequencies calculated analytically at using IFCs up to 9 <sup>th</sup>	neighbour at selected
points of the BZ for Pb. All frequencies are in THz	Z

Pb	Хт	XL	WT	WL	LT	$\mathbf{L}_{\mathbf{L}}$
EXP (a)	0.90	1.80	1.47	1.71	0.90	2.19
1-2N (c)	1.05	2.26	1.23	1.77	0.94	2.24
1-4N (c)	1.04	2.09	1.43	1.92	0.82	2.21
1-6N (c)	1.02	1.90	1.43	1.85	0.67	2.23
1-8N (b)	0.94	2.06	1.53	1.84	0.90	2.11
1-9N (c)	0.94	2.07	1.54	1.84	0.86	2.14

a Dal corso (2008)

b Cowley (1974)

c This work



### 3.2 PHONON DISPERSIONS OF PALLADIUM (Pd)



**Table3.2.1:** Frequencies calculated from quantum espresso at selected points of the bz forPd. All frequencies are in THz

Pd	a(a.u)	Хт	XL	WT	WL	LT	LL
EXP (a)	7.34	4.65	6.71	4.26	5.69	3.33	7.01
LDA(b)	7.30	5.12	7.17	4.37	6.01	3.58	7.38
GGA(b)	7.52	5.26	6.35	3.93	5.26	3.17	6.53

- a Miiller and Brockhouse (1971)
- b This work

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**Figure 3.2.2:** Calculated phonon dispersions for fcc-Pd from analytical approach using IFCs up to 9<sup>th</sup> neighbour

<b>Table3.2.2:</b> Frequencies calculated analytically using IFCs up to 9 <sup>th</sup> neighbour at selected
points of the BZ for Pd. All frequencies are in THz

Pd	Хт	XL	WT	$\mathbf{W}_{\mathbf{L}}$	$\mathbf{L}_{\mathbf{T}}$	$\mathbf{L}_{\mathbf{L}}$
EXP (a)	4.65	6.71	4.26	5.69	3.33	7.01
1-2N (c)	4.36	6.66	4.46	5.64	2.95	6.87
1-4N (c)	4.62	6.74	4.22	5.60	3.21	6.95
1-6N (c)	4.53	6.71	4.17	5.58	3.20	6.93
1-8N (b)	4.56	6.72	4.18	5.59	3.26	6.94
1-9N (c)	4.58	6.73	4.19	5.61	3.28	6.96

a Miller and Brochhouse (1971)

b Miller and Brockhouse (1971)

c This work

### **DISCUSSION OF RESULTS**

The phonon dispersion curves of the Fcc metals; Pb, and Pd, have been calculated using the Born-von Karman model with different numbers of interacting neighbours and exchange functional and the calculated values compared with experimental results. The different branches of the phonon band structure follow from the Eigen values after diagonalizing the dynamical matrix. The phonon frequencies in the first Brillouin zone were calculated along some high symmetry points and the current calculations show that from the gamma points, along the high symmetries  $R \rightarrow X$  and  $R \rightarrow L$  directions there are two branches of dispersion (Transverse and Longitudinal) which later split into three branches along the  $X \rightarrow W$  direction. By differentiating the phonon frequencies into two modes via acoustic longitudinal (LA) and Acoustic transverse (TA) at the Brillouin zone boundary, it is possible to characterize the high symmetry directions and identify which split corresponds to any of the modes.

### **Phonon Dispersion of Lead (Pb)**

The phonon dispersion of lead (Pb) calculated from quantum espresso code and interatomic force constant (IFCs) compared with experimental in elastic neutron scattering data (Dal Corso, 2008) are shown in Figures 3.1.1 and 3.1.2. The experimental inelastic neutron scattering is shown as black circles; the red line are the dispersions calculated by GGA functional while the green lines are the LDA dispersions. In the density functional theory calculations carried out for Pb, the electron - ion was treated using ultra soft and Projector Augmented Wave (PAW) (Audouze et al, 2008) as initio pseudo potential, within the applied self-consistent method. The calculations are carried out within the local density approximation (LDA) (Perdew and Zunger, 1981) and generalized gradient approximation GGA (Perdew et al, 1996) for the exchanged and correlation energy using Quantum espresso code (Gionnozzi, et al, 2009). The pseudo-wave functions are expanded in plane waves with a kinetic cut-off of 55Ryd for both LDA and GGA. The integration over the Brillouin zone were performed in the reciprocal space with uniform K-point meshes of 10 x 10 x 10 and 11 x 11 x 11 points for LDA and GGA respectively. The self-consistency calculation was assumed to have converged when the difference in energy between subsequent iteration was 1.0 x 10<sup>-3</sup> Ryds. Apparently Pb seems to be a relatively simple metal, with Fermi surface similar to free electron sphere perturb at Bragg planes by the lattice potential and several attempts to get its phonon dispersions with model pseudopotentials have been reported (Vosko et al, 1965; Bertoni et al, 1974). In practice even modern ab initio methods have found difficulties with the lattice dynamics of Pb due to the presence of several anomalies and to the small values of the interatomic force constants that make more evident the errors due to the numerical and physical approximations (Dal corso, 2008). In Brockhouse et al, (1962) it was observed that the interatomic force constants necessary to fit the Pb phonon dispersions extend to a large number of neighbours, a fact attributed to the large dips in phonon frequencies at the X point. In lead (Pb) at the equilibrium geometry the LDA functional gives phonon dispersions higher than experiment and GGA functional gives higher frequencies than experiment at the  $X_T$ ,  $W_L$ ,  $L_T$  points. At the  $X_L$ ,  $W_T$ , and L<sub>L</sub> points it is found to give phonon dispersions which are close to experiment. The

analytical calculated phonon dispersions of Pb using inter atomic force constants (IFCs) approach of the second (1-2NN), fourth(1-4NN), sixth(1-6NN), eighth(1-8NN), and ninth(1-9NN) nearest neighbour are shown in Figure 3.1.2 with the red lines, green lines, blue lines, purple lines and pink lines representing the 1-2NN, 1-4NN, 1-6NN, 1-8NN, and 1-9NN respectively. There negligible improvement in the quality of fit in the lead when the ninth neighbour (1-9NN) interactions were introduced. The phonon dispersions of the IFCs and LDA and GGA functional do not predict well the experimental phonons dispersions like other metals.

### Phonon Dispersions of Palladium (Pd)

The phonon dispersion of Palladium (Pd) results from quantum espresso code and interatomic force constant (IFCs) compared with experimental in elastic neutron scattering data (Miiller and Brockhouse, 1971) are shown in Figures 3.2.1 and 3.2.2. The experimental inelastic neutron scattering data are shown as black circles, the red line are the dispersions calculated by GGA functional while the green lines are the LDA dispersions. In the density functional theory calculations carried out for Pd, the electron-ion was treated using ultrasoft ab initio pseudopotential, within the applied self-consistent method. The calculations are carried out within the local density approximation (LDA) (Perdew and Zunger, 1981) and generalized gradient approximation GGA (Perdew et al, 1996) for the exchanged and correlation energy using Quantum espresso code. The pseudo-wave function is expanded in plane waves with a kinetic cut-off of 50Ryd and 45Ryd for LDA and GGA functional respectively. The integration over the Brillouin zone were performed in the reciprocal space with uniform K-point meshes of 10 x 10 x 10 for both LDA and GGA respectively. The self-consistency calculation was assumed to have converged when the difference in energy between subsequent iteration was  $1.0 \times 10^{-3}$  Ryd. The LDA phonon dispersions of palladium have been calculated at equilibrium lattice constant and an overestimation similar to other metals was found. Some previous papers (Grabowski et al, 2007; Stewart, 2008) confirmed this finding and are in good agreement with the results obtained in this research, but some other researchers also found good agreement with experiment at the LDA level. The GGA dispersions underestimate experimental results. Also the LDA underestimates the lattice constant by 0.5% while GGA overestimates it by 2.5%. The analytical calculated phonon dispersions of Pd using inter atomic force constants (IFCs) approach of the second (1-2NN), fourth(1-4NN), sixth(1-6NN), eighth(1-8NN), and ninth(1-9NN) nearest neighbour are shown in Figures 3.2.2 with the red lines, green lines, blue lines, purple lines and pink lines representing the 1-2NN, 1-4NN, 1-6NN, 1-8NN, and 1-9NN respectively. The analytical phonon dispersion curve of Pd shows that the second neighbour forces(1-2NN) gives lower frequencies at the transverse acoustic (T) branch about the X and L points, at the transverse acoustic (T) branch about the W point it is found to give a higher dispersion than experiment. The frequencies of the fourth(1-4NN), sixth(1-6NN), eight(1-8NN) and ninth(1-9NN) neighbour forces are closer to experimental results than those of Quantum espresso code.

### CONCLUSION

For all the metals studied in this research the local density approximation (LDA) gives phonon dispersion slightly higher than experimental results while the generalized gradient approximation (GGA) gives slightly lower frequency.

For Pb it was observed that the extension to  $1-9^{th}$  neighbor gave slightly close agreement with the experimental phonon dispersions when compared to the  $1 - 8^{th}$  neighbor at some symmetry points. Pb at point  $L_L$  gave percentage errors of 2.2% and 3.6% for  $1 - 9^{th}$  and  $1 - 8^{th}$  neighbours respectively. The phonon dispersion curve of lead shows that the inter-atomic forces are of very long-range nature. The Force constant for neighbor more distant than the fourth neighbor has distinctly smaller values.

It has been shown for the first time that by extending our calculation from first to ninth neighbour for Pb, and Pd, there is an improvement in the phonon dispersion curve when compared with first to eight and fit to fifth neighbours of other researchers respectively.

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