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

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ABSTRACT.

The Computational theoretical techniques was applied in the investigation of Phonon Dispersion of Lead (Pb) and Palladium (Pd).

The first principle technique which make use of the density functional theory as implemented by quantum expresso as well as inter – atomic force constant (IFC) techniques (Born-von Jarman) which was extended to higher number of neighbours than what is available in the literature were employed in this research.

The results obtained shows that the local density approximation (LDA) phonon dispersion slightly overestimates experimental results whereas the generalized gradient approximation (GGA) gives slightly lower frequency. However, there was negligible improvement in the quality of fit in lead when the ninth neighbour (1 - 9NN) interaction were introduced.

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

1.0 INTRODUCTION

The physical properties of Lead(Pb) and Palladium(Pd) are of strong scientific interest – fundamentally as a highly correlated electronic system and technologically. The role of palladium in hydrogen storage and nanoscale materials has continue to attract both theoretical and experimental interests. The low power requirement and fast response exhibited by Pd nanowires in the area of hydrogen sensors has contributed to the advancement of sensor technology.

Experimentally, Pd has shown large scale device integration in nanoscale applications, and has also exhibited interesting magnetic properties.

Stewart (2008) in his research used density functional perturbation theory (DFPT) to examine the acoustic characteristics that were reserved for electronic properties. The usefulness of lead in Cable sheathing, radiation protection, batteries etc as a constituent of solder type metal, pewter, beaming and fusible alloys are in wide applications.

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).

The results of experiments on thermal diffuse x-ray scattering experiments (Burkel *et al*, 1987; Dorner *et al*, 1987) and inelastic neutron scattering experiments (Kazanc and Ozgen 2008) shows lattice vibration frequencies.

The challenges of theorists is to solve 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 using the dynamical matrix generated. (Bencherif *et al*, 2011; Ruf *et al* 2001).

The two main theoretical techniques are the ab – initio (or first principles methods) and empirical (or phenomenological) (Baroni *et al*, 2001).

Srivastava, (1990) observed that the challenge of the empirical (or phenomenological) is its inapplicability in all types of solids while Dreizler and Gross,(1990) and Martin (2004) argued that the ab – initio (or first principles methods) is unsuitable for the the investigation of ground state properties of excited systems.

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 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.

2.0 THEORETICAL CALCULATION AND CONSIDERATIONS

2.1 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)

$$\mathrm{H}\psi(r_i - - - r_{n,}R_i - - - R_N) = \varepsilon\psi(r_i - - - r_{n,}R_i - - - R_N) \tag{2.1}$$

Where Ψ is the wave function, ε 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

$$H = -\sum_i \frac{h^2\partial^2}{2m\partial r_l^2} - \sum \frac{h^2\partial^2}{2m\partial r_i^2} + \sum_{i>j} \frac{e^2}{|r_i - r_j|} + \sum V_b(r_l - R_{l'}) + \sum_{l,i} V_b(r_i - R_l) \tag{2.2}$$

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 pair-wise bare ion-ion interaction. While the fifth term is the bare ion-electron interaction $\substack{r_{i}-r,\\ R_i - R,}$

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

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

$\mathrm{E}_n(R)$, 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:

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

If the ion Hamiltonian is

$$H_i = -\sum_i \frac{h^2\partial^2}{2m\partial r_l^2} + \sum V_b(r_l - R_{l'}) \tag{2.5}$$

We then add $\mathrm{E}_n(R)$ to it and put the total wave function to solve the Schrödinger equation

$$H = \left\{-\sum_i \frac{h^2\partial^2}{2m\partial r_l^2} + \sum W_b(r_l - R_{l'}) + \mathrm{E}(R)\right\}\psi_n(r,R)x(R) = \mathrm{E}\psi_n(r,R)x(R) \tag{2.6}$$

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

$$\left\{-\sum_l \frac{h^2\partial^2}{2\mathrm{M}\partial R_l^2} + \sum_{l>l'} W_b(R_l - R_{l'}) + \mathrm{E}_n(R)\right| x(R) = Ex(R) \tag{2.7}$$

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

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

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

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

Where n_e is the total number of electrons and $\frac{\partial n_e}{\partial R_l}$ = 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

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

(2.10) Equation (2.10) is the product of m/M and the kinetic energy of the electron in its motion round the ion at R_l. This is small since 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.

2.2 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 " α direction when the atom moves a unit distance in the " β direction. The force constant matrix $\phi_{\alpha\beta}(0,l)$ is symmetric. l_1, l_2, l_3 are three non-negative integers with $l_1 \geq l_2 \geq l_3$. 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.

3.0 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.

3.1 PHONON DISPERSIONS OF LEAD(Pb)

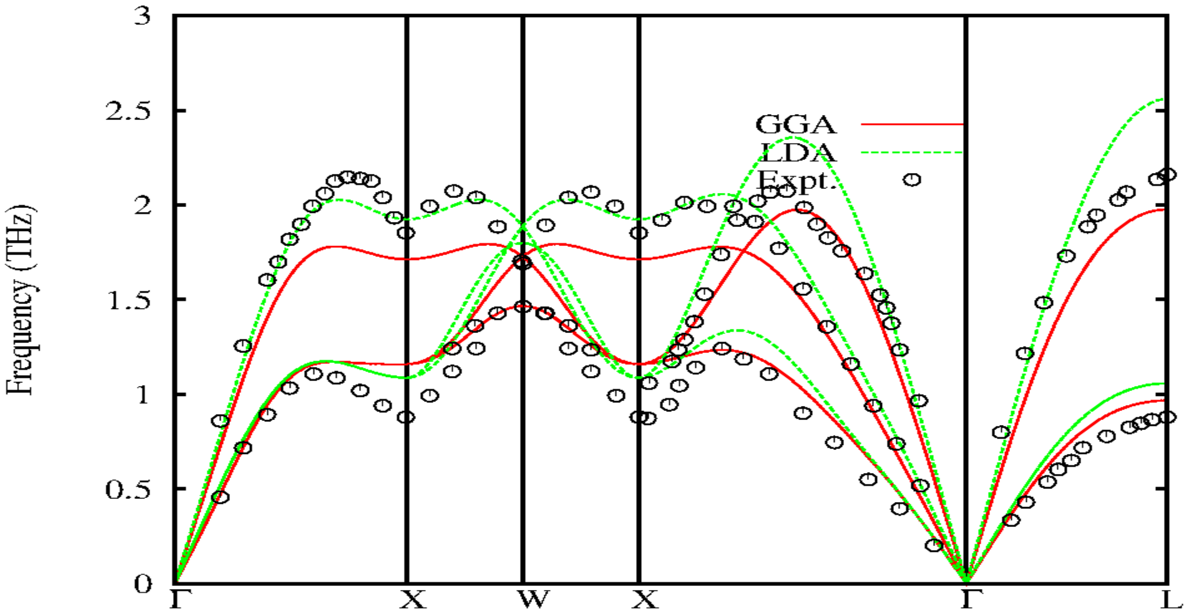

Figure 3.1.1: Calculated phonon dispersions for fcc-Pb compared to inelastic neutron scattering data (black circles) Dal corso (2008)

Table3.1.1: Frequencies calculated from quantum espresso at selected points of the BZ for Pb. All frequencies are in THz

Pb	**a(a.u)**	**X_T**	**X_L**	**W_T**	**W_L**	**L_T**	**L_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

a Dal corso (2008)

b This work

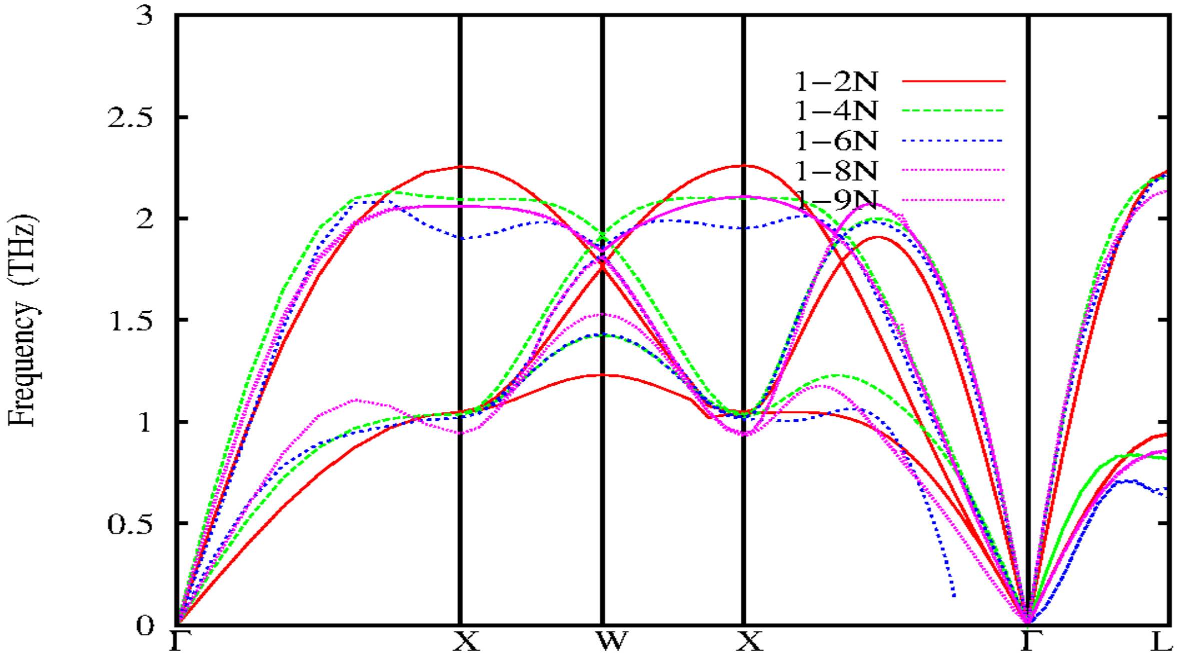

Figure 3.1.2: Calculated phonon dispersions for fcc-Pb from analytical approach using IFCs up to 9th neighbour

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

Pb	**X_T**	**X_L**	**W_T**	**W_L**	**L_T**	**L_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)

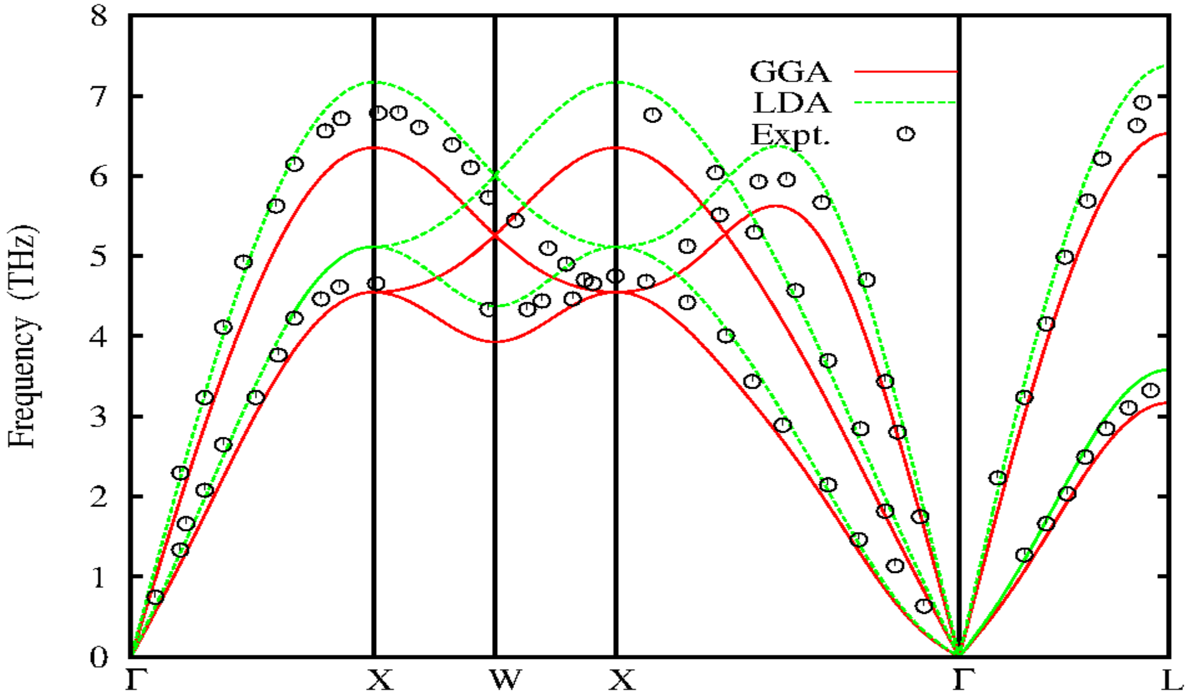

Figure 3.2.1: Calculated phonon dispersions for fcc-Pd compared to inelastic neutron scattering data (black circles) Miiller and Brockhouse (1971)

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

Pd	**a(a.u)**	**X_T**	**X_L**	**W_T**	**W_L**	**L_T**	**L_L**
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

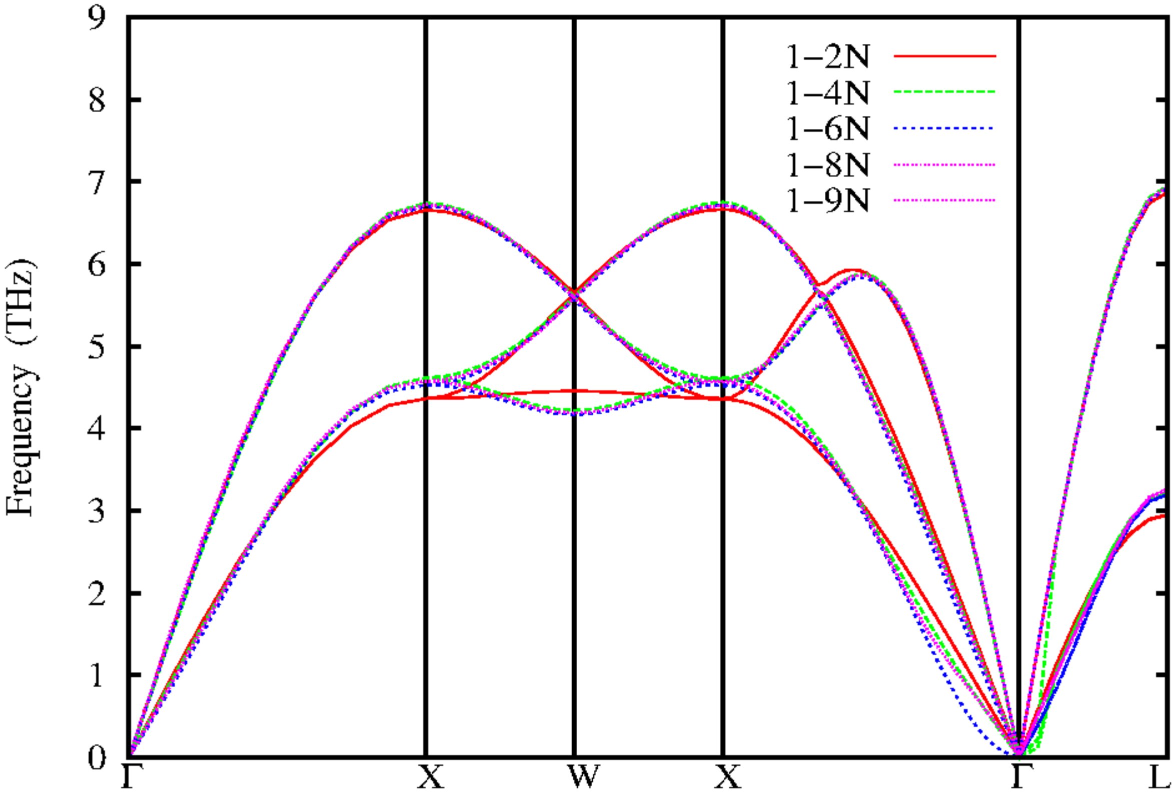

Figure 3.2.2: Calculated phonon dispersions for fcc-Pd from analytical approach using IFCs up to 9th neighbour

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

Pd	**X_T**	**X_L**	**W_T**	**W_L**	**L_T**	**L_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

4.0 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.

4.1 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. 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 1.0×10^{-3} Ryds. The GGA functional gives higher frequencies than experiment at the $X_{T,}$ $W_{L,}$ L_T points. At the $X_{L,}$ $W_{T,}$and L_L 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.

4.2 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. 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 has 50Ryd and 45Ryd for LDA and GGA functional respectively. The integration over the Brillouin zone were performed in the reciprocal space with 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 x 10^{-3} Ryd and 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. The GGA dispersions underestimate experimental results. Also twe observed 0.5% underestimation for LDA 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.

5.0 CONCLUSION

For all the metals studied in this research the LDA gives phonon dispersion slightly higher than experimental results while the GGAgives slightly lower frequency.

For Pb it was observed that the extension to 1-9th neighbor gave slightly close agreement with the experimental phonon dispersions when compared to the 1 – 8th neighbor at some symmetry points. Pb at point $\mathbf{L}_L$ gave percentage errors of 2.2% and 3.6% for 1 – 9th and 1 – 8th 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.

REFERENCES

Audouze, C., Jollet, F., Torrent, M., and Gonz, X. (2008) Comparison between projector Augmented – wave and ultra – soft pseudopotential formalisms at the density functional perturbation theory leve. Phy. Rev. B. 78, 035105

Baroni S., deGironcoli S., Dal CorsoA., and Giannozzi P (2001). Phonons and related crystal properties from density-functional perturbation theory. Rev Mod Phys **73**: 515-562

Bencherif, Y., Boukra, A., Zaoui, A, and Ferhat, A. (2011). Lattice dynamics study of lead chalcogenides. Elsievier Infra red physics and Technology **54**, 39 – 43.

Bertoni, C. M, Bortolani, V, Calandra, C., and Nizzoli, F (1974). Third order perturbation theory and lattice dynamics of simple metals. J. Phys. F. Met. Phys. 4, 19

Born M., and Huang K. (1954). Dynamical Theory of Crystal lattice (Oxford University Press, London).

Born M., and Oppenheimer, J. K. (1927). On the quantum theory of molecules. Ann. Physik 84, 457

Brockhouse B.N.,Arase T, Caglioti G., Rao R. K., and Woods A.D.B (1962). Crystal Dynamics of Lead I. Dispersion Curves at 100°k.Phys. Rev. Vol. 128pp. 1099.

Burkel, E., Peisl, J., and Dorner, B. (1987). Observation of inelastic x – ray scattering from phonons. Europhys Lett. 3, 957 – 961.

Dal corso, A. (2008) Ab initio phono dispersions of face center cubic Pb: Effect of spin orbit coupling. J. Phys.: Cond. Matter 20. 445202

Dorner, B., Burkel, E., Illini, Th., and Peisl, J., (1987). First measurement of a phonon dispersion curve by inelastic x – ray scattering. Phys. B. 69, 179 – 183.

Cowley E. R. (1974). A Born-Von Karman Model For Lead. Solid state comm, vol. 14, 587-589

Dreizler, R. M., and Gross, E.K.U., (1990). Density Functional Theory: An approach to the Quantum many – body problem. Springer, Berlin Germany.

Einstein, A (1905) The motion of elements suspended in static liquids as claimed in molecular kinetic theory of heat. Annalen der Physik 17, 549 – 560.

Einstein, A (1906). A new determination of the molecular dimensions. Annalen der Physik 19, 289 – 306.

Einstein, A (1907). The Planck theory of radiation and the theory of specific heat. Annalen der Physik 22, 180 – 190.

Enaroseha O. E. Omamoke and E. G. Akpojotor (2013). Superconductivity Driven by Magnetic Instability in $CeCu_2Si_2$. Advances in Physics Theories andApplication, Vol.18, 54 – 60.

Enaroseha O. E. Omamoke, Obed Oyibo, and N. Okpara. (2021). Analysis of Ground State Properties of Interacting Electrons in the Anderson Model. The Journal of Applied Sciences Research, 8(1), 15 – 27.

Enaroseha O. E. Omamoke, Obed Oyibo, Damaris Osiga – Aibangbee and Eno Odia (2021). Magnetic Phase Diagram in the Periodic Anderson Model (PAM): An Exact Diagonalization Approach. International Research Journal of Pure and Applied Physics, Vol. 8(1): 14 – 21

Enaroseha O. E. Omamoke and N. N. Omehe (2020). Heat Transfer in Circular Tubes with Supercritical Fluid Using the STAR CCM + CFD Code, African Journal of Research in Physical Science 10, 24 – 31.

Enaroseha, O. E Omamoke, Priscilla O. Osuhor, Obed Oyibo And Ernest O. Ojegu (2021). Theoretical Study of Phonon Spectra in Aluminium (Al) and Copper(Cu): Application of Density Functional Theory and Inter– Atomic Force Constant. Solid State Technology Volume: 64 (2), 1984 - 1999

Enaroseha, O. E Omamoke, Obed Oyibo, Priscilla O. Osuhor, Ovie Oghenerhoro (2021). Lattice Dynamics in Some FCC Metals: Application of Phonon Dispersions in Nickel (Ni) and Platinium (Pt). Solid State Technology Vol. 64(2), 4640 - 4655

Omehe N. N. and Enaroseha, O. E Omamoke (2019). Ab Initio Investigation of $AgGa_2$ and $AgGaSe_2$. International Journal of Engineering Applied Sciences and Technology, 4 (5), 354 – 360

Enaroseha O. Omamoke, O Oyibo, Augustine O. Nwabuoku and Blessing Odia Ogo (2022) Single and Multi– Phase Dynamics of the(Anti)Ferromagnetic CeCu2Si2 Systems. Neuroquantology Vol. 20(14), 644 – 649

Enaroseha O. E. Omamoke, Obed Oyibo, Oghenevovwero E. Esi, Edward O. Tuggen and Jennifer A. Nomuoja (2023) The First Principle Calculation of the Properties of Aluminium and Gallium Using Density Functional Theory. European Chemical Bulletin, Vol. 12(5), 290 – 297. Retrieved from Research Square at https://doi.org/10.21203/rs.3.rs-3102806/v1

Gionnozzi P., Baroni S., Bonini N., Calandra M., Car R., Cavazzoni C.,Ceresol D., Chiarotti G., Cococcioni M., Dabo I., Corso A., de Goroncoli S., Fabris S.,Gebauer R., Gerstmann U., Gougoussis C., Kokalj A., Lazzeri M ., Martin- samos L., Marzari N., Mauri F., Mazzarello R., Paolini S., Pasquarello A., Paulatto L., Sbraccia C., Scandolo S., Sclauzero G., Seitsonen A P., Smogunov A., Umari P., Wentzcovitch R.M.,(2009) QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. J Phys. Cond. Matter 21(39): 395502

Grabowski G., Hickel T., and Neugebauer J.,(2007). Ab initio study of the thermodynamic properties of non-magnetic elementary fcc metals. Exchange-correlation-related error bars and chemical trends. Phys. Rev. B. 76 024309.

Kazanc S., and Ozgen S., (2008). An Investigation of Temperature effect on a phonon dispersion spectra of Ni by Molecular Dynamics simulation. Turk.J.Phys. 32, 315-322.

Kittel C. (1996). Introduction to Solid State Physics, 7th edition. John Wiles &Sons, New York.

Lin. G. (2005). Investigation of properties in barium chalcogenidea from first principles calculations. Unpublished Ph.D Thesis submitted to the Department of Physics, Federal University of Agriculture, Abeokuta.

MartinR.M.(2004). Electronic Structure: Basic theory and practical methods. Cambridge University press United Kingdom, 1st edition pg173.

Miller A.P.,and Brockhouse B.N. (1971). Crystal dynamics and electronic specific heat of palladium and Copper. Canadian Journal of Physics, 49, 704 – 723.

Perdew J. P and Zunger A., (1981). Self-Interaction Correction to density-functional approximation for many-electron systems. Phys. Rev. B 23, 5048

Perdew J.P., Burke, K., and Ernzerhof M.,(1996). Generalized Gradient Approximation Made Simple. Phys. Rev. Lett. 77, 3865

Ruf, T., Serrano, J., Cardona, M., Pavone, P., Pabst, M., Suski, T., and Leszczynski (2001). Phonon dispersion curves in Wurtzite – structure GaN: Determined by x – ray scattering. Phy. Rev. Lett. 86, 906 – 909.

Slater, J. C. (1963). Quantum theory of molecules and solids. McGraw - Hill

Srivastava G. P (1990). The Physics of Phonons, Hilger, Bristol

Stewart, D. A (2008). Ab – initio investigation of phonon dispersion and anomalies in Palladium. New J. of Phy. 10, 043025 – 043033.

Vosko S.H., Taylor R., and Keech G.H. (1965). The influence of the Electron-ion interaction on the phonon frequencies of simple metals Na, Al, and Pb. Can. J. Phys. 431187.

Ziman, J. M. (1965). Principles of the theory of solids. American Journal of Physics 33, 349.