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Article

Phonon Dispersion Curves of Silver (Ag) and Gold (Au): Application of Density Functional Theory and Inter – Atomic Force Constant

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Abstract: The Computational theoretical techniques using first principle 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) were used to investigate the phonon dispersion curves of Silver (Ag) and Gold (Au). The results obtained show that for Au, the extension to 1 – 6th neighbour gave slightly close agreement with the experimental phonon dispersions when compared to the 1 – 5th neighbor at W_T and L_L symmetry points. The percentage error for Au at W_T are 2.5% and 2.9% ; at point L_L we obtained 0.6% and 0.7% respectively. The Local density Approximation (LDA) results for Ag underestimates the lattice with about 1.6% while the Generalized Gradient Approximation (GGA) overestimates it by 1.9%.

Keywords: phonon; quantum expresso; Eigen – value; silver (Ag); gold (Au)

1.0 Introduction

The measurement of phonon-dispersion curves in the symmetry directions and then fitting force-constant models to the measured frequencies has been a subject of interest for many years in the studies of the lattice dynamics of metals. The force constants are assumed to have a physical meaning sometimes they are used only as a means of obtaining interpolation formulas for the calculations of phonon frequencies distributions and polarization vectors (Nilsson and Rolandson, 1973). By assuming certain conditions for the relations between some of the constants, one may include good fit forces from remote neighbour and derive curves to give a very good fit in measured direction.

Theoretical calculations of the lattice dynamics of metals have been attempted from first principles by a number of authors (Toya 1964; Vosko *et al*, 1965; Harrison 1966). None of these has had marked success except for the alkaline metals. However, Harrison (1966) has shown how a Pseudopotential can be derived from a phenomenological model involving only two free parameters which can be evaluated from phonon measurements.

Force constant analysis of the data for Pb has generally proved a failure. Models of several kinds with forces going out as far as the tenth neighbour have been tried without success. Indeed there is reason to believe that forces could extend to twenty neighbours (Brockhouse *et al* 1962).

Hanke (1971) used the shell model to discuss the dynamics of Cu, Ni and some other metals, his idea was to use the shell-core concept to simulate polarization effects in the noble and transition metals. While the use of dipolar model for metals first seem inappropriate, Hanke has argued that the applicability of the model can be made plausible by microscopic consideration (Venkataraman *et al*, 1974).

The aim of this research is to obtain the phonon dispersions curves of two Face Centered Cubic (FCC) metals namely Silver (Ag) and Gold(Au) from accurately determined interatomic force

constants (IFCs) using quantum espresso code as implemented by Gionnozzi *et al* (2009), IFC approach up to at least sixth neighbour and compare phonons results with experimental data.

2.0 Theoretical Calculation and Considerations

2.1 Normal Mode Frequencies in Three Dimensions

Every type of lattice has its own characteristic mode or frequencies of vibration called normal modes. In three dimension, for a mass m at the origin 0 , the equation of motion corresponding to the displacement of atom $u(l)$ can be generalized as

$$f_o = \sum_l \varphi(l) \cdot \ddot{u}(l) \quad (2.1)$$

If we use α and β as coefficient to represent the Cartesian components of the vectors, the force equation (2.3) can be written as:

$$F_{\alpha\beta} = - \sum_l \sum_{\beta=1} \varphi_{\alpha\beta}(l) u_{\beta}(l) \quad (2.2)$$

$$\alpha = 1, 2, 3$$

(The minus sign is introduced simply for convenience).

There are now three equation of motion for each atom, corresponding to the three degree of freedom.

$$F_o = \frac{m \partial^2}{\partial t^2} U_{o,\alpha} = - \sum_l \sum_{\beta=1} \varphi_{\alpha\beta}(l) u_{\beta}(l) \quad (2.3)$$

And the three- dimensional form of a plane wave is

$$U_{l,\alpha}(q) = A_{\alpha} \exp[i(\omega t - q \cdot r_l)] \quad (2.4)$$

Therefore equation (2.5) becomes

$$-m\omega^2 A_{\alpha} \exp(i\omega t) = - \sum_l \sum_{\beta=1}^3 \varphi_{\alpha\beta}(l) A_{\beta} \exp[i(\omega t - q \cdot r)] \quad (2.5)$$

To facilitate the generalization to a limit cell containing more than one atom, it is convenient to make two new definitions at this point.

$$B = m^{\frac{1}{2}} A_{\alpha}, D_{\alpha\beta} = \frac{1}{m} \sum_l \varphi_{\alpha\beta}(l) \exp(-iq \cdot r_l) \quad (2.6)$$

Substituting equation (2.8) into (2.7) becomes

$$M^{\frac{1}{2}} A_{\alpha} \omega^2 = \frac{1}{m} \sum_l \sum_{\beta=1}^3 \varphi_{\alpha\beta}(l) A_{\beta} \exp(-iq \cdot r_l) * m^{\frac{1}{2}} \quad (2.7)$$

$$\omega^2 B_{\alpha} = \sum_{\beta}^3 D_{\alpha\beta} B_{\beta}, \alpha = 1, 2, 3 \quad (2.8)$$

Or in the matrix form

$$\omega^2 B = D \cdot B \quad (2.9)$$

This is a typical eigenvalue problem and the solutions for ω^2 are the roots of the determinant equation.

D in equation (2.10) is known as the dynamical matrix, and the determinant is called the secular determinant (Venkataraman, *et al*, 1974).

$$D(q) - \omega^2 I \nabla 0 \quad (2.10)$$

Equation (2.10) is obtained from the equation (2.9) and the roots $\omega^2(q)$ are the Eigen-values of $D(q)$. In general, the dynamical matrix for a lattice with basis of n atoms has $3n \times 3n$ dimensions which assumes the general form

$$D_{\alpha\beta}(q) - m\omega^2 I \partial_{\alpha\beta} \nabla 0 \quad (2.11)$$

Where $D_{\alpha\beta}(q)$ are elements of the dynamical matrix, q is the wave-vector confined to the first Brillouin zone; I is a limit matrix of order α and β and m is the ionic mass (Born and Huang; 1954).

In more explicit terms, equation (2.12) may be written as:

$$(D_{xx} - m\omega^2 D_{xy} D_{xz}) (D_{yz} D_{yy} - m\omega^2 D_{yz}) \quad (2.12)$$

$e_x(q), e_y(q)$ and e_z are unit polarization vectors which satisfy the orthogonality condition that

$$e_{\alpha}(q) e_{\beta}(q) = \partial_{\alpha\beta} \quad (2.13)$$

Where

$$\partial_{\alpha\beta} = \{1 \text{ if } \alpha = \beta\} \quad (2.14)$$

Equation (2.13) is the matrix representation of the expression that will be required to solve in order to determine the phonon dispersion relations $[w_p(q) \text{ for } p = 1, 2, 3]$ in the symmetry

directions [100], [110] and [111] in a cubic crystal. The dynamical matrix is given in equation (2.4). In a metal, there are three contributions to the dynamical matrix $D_{\alpha\beta}$ associated with the effective potential between the ions. These contributions are the columbic $D_{\alpha}^{C\beta}$, the Born-mayer $D_{\alpha}^{R\beta}$, and the electronic band structure, $D_{\alpha}^{E\beta}$, contributions, respectively (Animalu, 1977). The columbic contribution arises from the long-range columbic interaction between bare ions. The repulsive Born-Mayer contribution is associated with ions and it arises from the overlap of the core electron wave function on neighboring. The electronic contribution is associated with the indirect ion – electron – ion interaction via the polarization field of the conduction or valence electrons.

The electronic contribution depends on the Pseudo-potential carried rigidly by the ions, i.e on the electron-phonon coupling matrix (Sham and Ziman, 1963).

We may then write $D_{\alpha\beta}$ notionally as a sum of the three components i.e

$$D_{\alpha\beta} = D_{\alpha}^{C\beta} + D_{\alpha}^{R\beta} + D_{\alpha}^{E\beta} \quad (2.15)$$

While the first two contributions can be handled in real space, the last component is more conveniently handled in the reciprocal lattice space. (Okoye 2002).

The phonon frequencies w^2 are obtained when the elements of the dynamical matrix are substituted in equation (2.8). On solving equation (2.8) three homogeneous equations in three unknowns equations, $w_p(q)$ ($p = 1, 2, 3$) are obtained. The solutions corresponding to $w_p(q)$ are determined by finding the roots of the determinant equation in equation (2.9); these roots determine the phonon frequencies. If the value of $w^2 p$ is negative the value of w_p becomes imaginary and the atomic motion increases exponentially with time, thus causing instability in the crystal structure. Also, if the phonon frequency is reduced and eventually comes to zero, then such a mode is called soft phonon mode (Srivastava, 1990). The presence of a soft mode crystal deforms the original crystal structure in favour of a more stable structure (Baroni *et al*, 2001).

In our recent work we studied Lattice Dynamics in some FCC Metals using the following metals Nickel (Ni) and Platinum (Pt) Enaroseha *et al* (2021a); Aluminium (Au) and Copper (Cu) Enaroseha *et al* (2021b); and Lead (Pb) and Palladium (Pd) Enaroseha *et al* (2021c) as well as AgGaS₂ and AgGaSe₂ (Omehe and Enaroseha)

2.2 Analytical Procedure

The application of the Born-von Karman theory (Born and Huang, 1954; Enaroseha *et al*, 2023) to fcc lattices have been described by many authors. Ag and Au belong to the space group of O_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 $\varphi_{\alpha\beta}$ 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 $\varphi_{\alpha\beta}(0, l)$ 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: Ag and Au 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 Ag are presented in section 3.1 while the results of the phonon dispersion relation for Au from inter – atomic force constants (IFCs) approach and quantum espresso code are presented in section 3.2.

3.1 Phonon Dispersions of Silver (Ag)

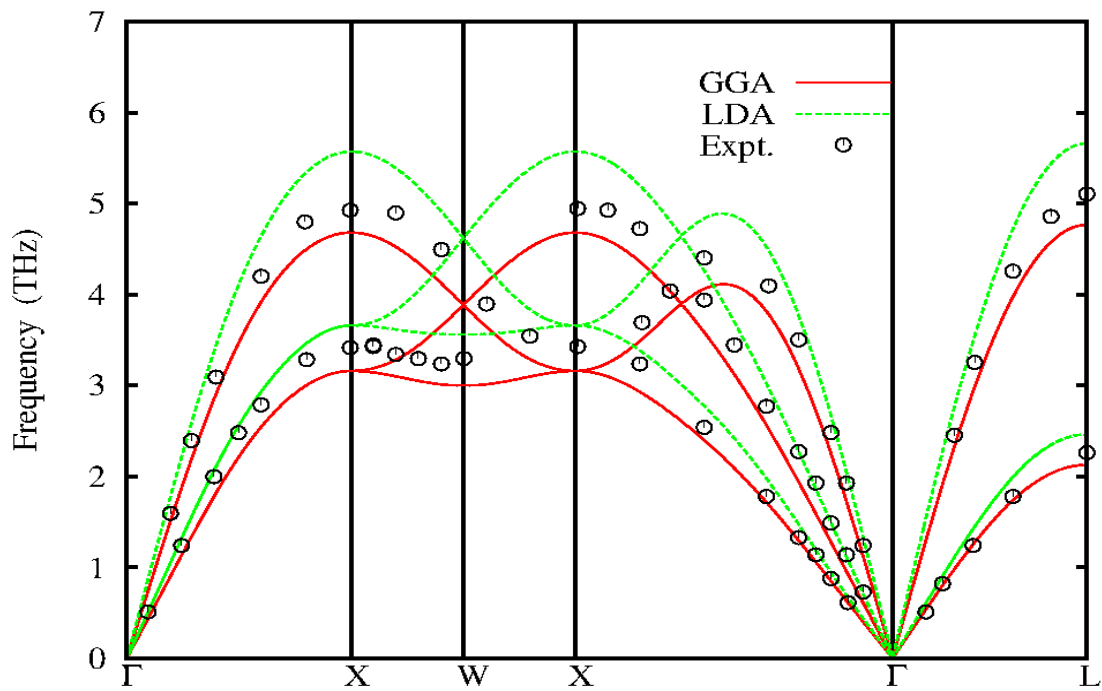


Figure 1. Calculated phonon dispersions for fcc-Ag compared to inelastic neutron scattering data (black circles) Kamitakahara and Brockhouse(1969).

Table 1. Frequencies calculated from Quantum espresso at selected points of the BZ for Ag. All frequencies are in THz.

Ag	a(a.u)	X _T	X _L	W _T	W _L	L _T	L _L
EXP (a)	7.72	3.41	4.94	3.29	-	2.31	5.09
LDA(b)	7.60	3.66	5.57	3.56	4.62	2.46	5.66
GGA(b)	7.89	3.16	4.68	3.00	3.89	2.13	4.77

a. Kamitakahara and Brockhouse(1969); b. This work.

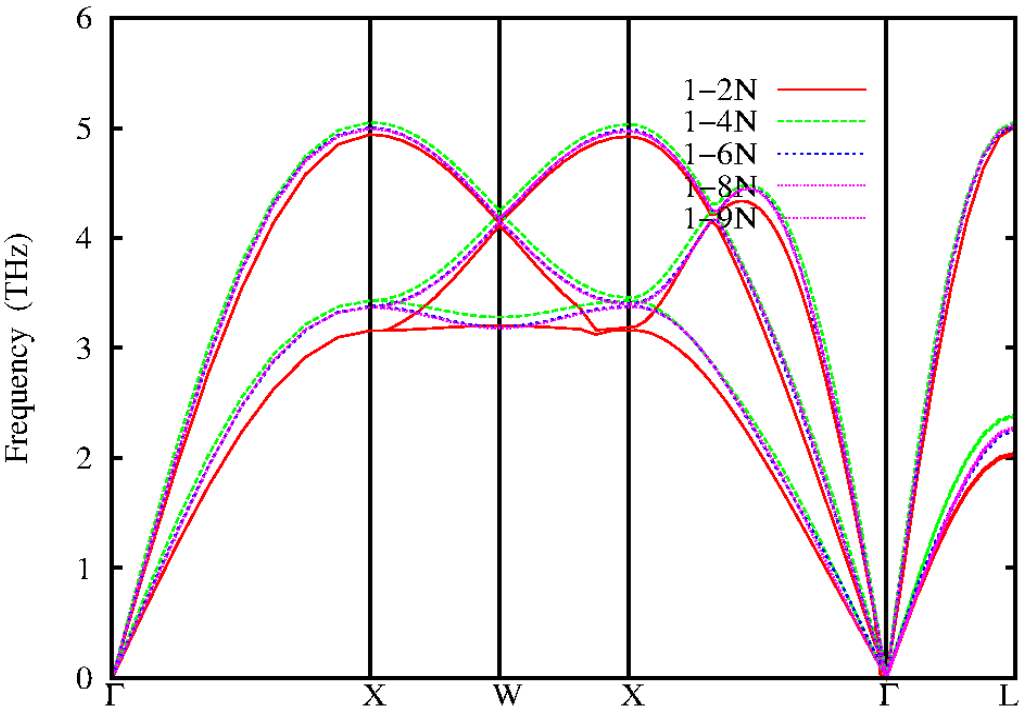


Figure 2. Calculated phonon dispersions for fcc-Ag from analytical approach using IFCs up to 9th neighbour.

Table 2. Frequencies calculated analytically using IFCs up to 9thneighbour at selected points of the BZ for Ag. All frequencies are in THz.

Ag	X _T	X _L	W _T	W _L	L _T	L _L
EXP (a)	3.42	4.95	3.29	-	2.31	5.09
1-2N (c)	3.16	4.94	3.20	4.14	2.04	5.02
1-4N (c)	3.43	5.05	3.28	4.24	2.39	5.06
1-6N (c)	3.38	5.01	3.19	4.17	2.26	5.02
1-8N (b)	3.37	5.00	3.17	4.18	2.28	5.04
1-9N (c)	3.38	4.97	3.18	4.19	2.30	5.07

a. Kamitakahara and Brockhouse (1969); b. Dutton *et al* (1972); c. This work.

3.2 Phonon Dispersions of Gold (Au)

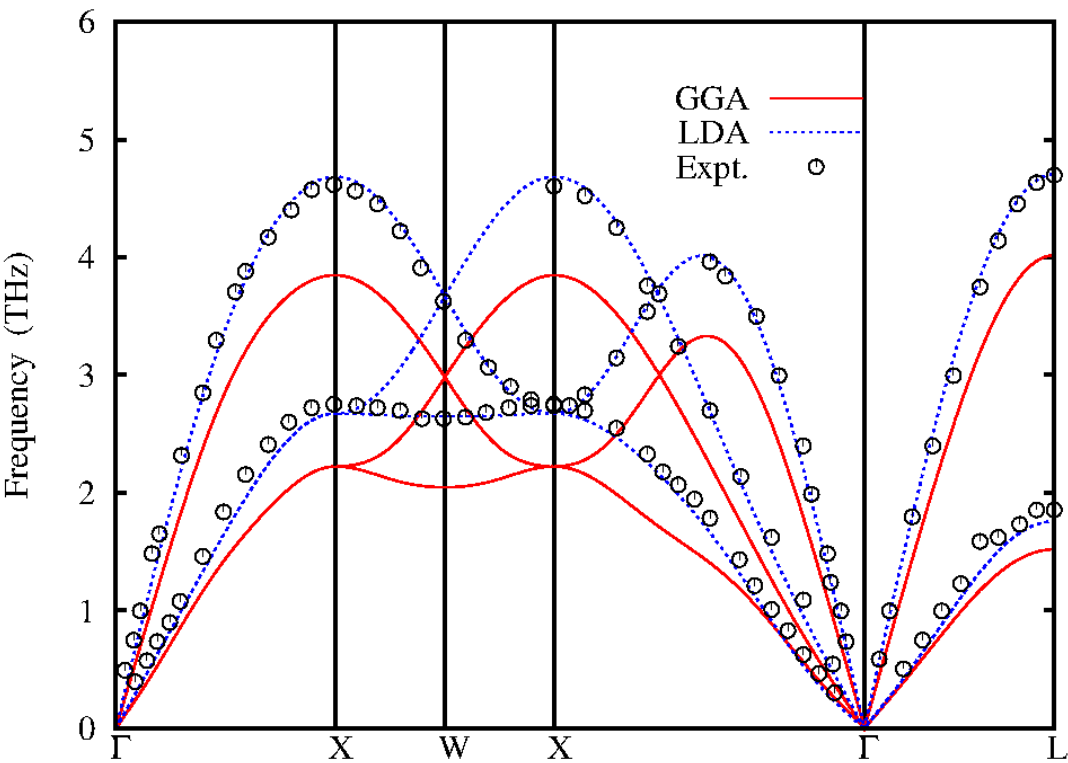


Figure 3. Calculated phonon dispersions for fcc-Au compared to inelastic neutron scattering data (black circles) Lynn *et al* (1973).

Table 3. Frequencies calculated from Quantum espresso at selected points of the BZ for Au. All frequencies are in THz.

Au	a(a.u)	X _T	X _L	W _T	W _L	L _T	L _L
EXP (a)	7.34	2.76	4.61	2.64	3.63	1.86	4.71
LDA(b)	7.65	2.67	4.68	2.65	3.67	1.76	4.71
GGA(b)	7.90	2.22	3.85	2.05	2.98	1.52	4.02

a. Lynn *et al* (1973); b. This work.

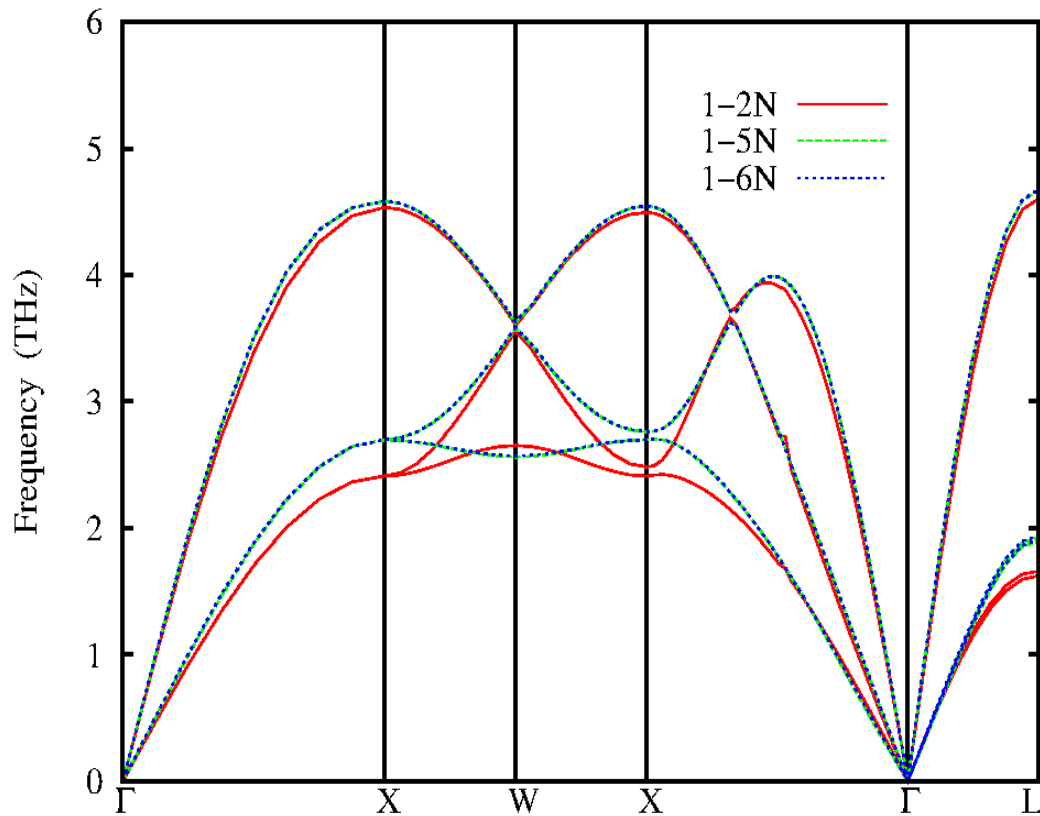


Figure 4. Calculated phonon dispersions for fcc-Au from analytical approach using IFCs up to 6th neighbour.

Table 4. Frequencies calculated analytically using IFCs up to 6thneighbour at selected points of the BZ for Au. All frequencies are in THz.

Au	X _T	X _L	W _T	W _L	L _T	L _L
EXP(a)	2.76	4.62	2.64	3.63	1.86	4.71
1-2N(c)	2.41	4.53	2.65	3.60	1.64	4.62
1-5N(b)	2.70	4.59	2.59	3.62	1.90	4.67
1-6N(c)	2.71	4.60	2.57	3.63	1.91	4.68

a. Lynn et al (1973); b. Lynn et al (1973); c. This work.

4.0 Discussion of Results

The phonon dispersion curves of the Fcc metals; Ag, and Au, 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→X and R→L directions there are two branches of dispersion (Transverse and Longitudinal) which later split into three branches along the X→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.

4.1 Phonon Dispersion of Silver (Ag)

The phonon dispersion of Silver (Ag) calculated from Quantum Espresso code (Gionnozzi *et al*, 2009) and inter atomic force constants (IFCS) compared with experimental inelastic neutron scattering data (Dal corso, 2013) are shown in Figures 1 and 2. The experimental inelastic neutron scattering are shown as black circle, redlines are the dispersion calculated by Local Density Approximation (LDA) functional. In the Density Functional Theory (DFT) carried out for Ag, the electron-ion was treated using norm conserving ab – initio pseudopotential, within the applied self-consistent method. The calculations are carried out within the LDA (Perdew and Zunger, 1981) and Generalized Gradient Approximation (GGA) (Perdew *et al*, 1996) for the exchange and correlation energy using Quantum espresso code. The pseudo-wave functions are expanded in plane waves with kinetic energy cut of 45Ryd for both LDA and GGA. The integration over the Brillouin zone was performed in the reciprocal space with Uniform K-point meshes of 12 X 12 X 12 points for both LDA and GGA. The self-consistency calculation was assumed to have converged when the difference in energy between subsequent iteration was 1.0×10^{-3} Ryd. In silver, some researchers (Grabowski *et al*, 2007; Xie *et al*, 1999) have reported in their work that the LDA functional gives higher phonon frequencies while GGA functional suffers over determination, giving too low frequencies. This is in agreement with the results obtained in this work as shown in Table 1. The LDA underestimates the lattice of about 1.6% while the GGA overestimates it by 1.9%. The analytical calculated phonon dispersions of Ag using IFCS approach of the 1-2NN, 1-4NN, 1-6NN, 1-8NN and 1-9NN (NN means Nearest Neighbour) are shown in Figure 2 with red lines, green lines, blue lines, purple lines and pink lines representing the nearest neighbours respectively. The analytic phonon dispersion curve of Ag shows that the second neighbour forces (1-2NN) underestimate the experimental except at the longitudinal acoustic branch L about the W point where the frequency is close to experimental results. The frequencies of the 1-4NN, 1-6NN, 1-8NN and 1-9NN gives a better prediction of the experimental phonon dispersion than those of the LDA and GGA functional from Quantum Espresso Code..

4.2 Phonon Dispersion of Gold (Au)

The phonon dispersion of Au calculated from quantum espresso code and inter atomic force constants (IFCs) compared with experimental inelastic neutron scattering data (Lynn *et al*, 1973) are shown in Figures 3 and 4. The experimental inelastic scattering data are shown as black circles, the red line are the dispersions calculated by GGA functional while the green lines are the LDA dispersion. The density functional theory (DFT) calculations carried out for Au, the electron-ion was treated by using ultra soft 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 exchange and correlation energy using quantum espresso code. 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 11 x 11 x 11 and 12 x 12 x 12 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} Ryd. In gold (Ag) the phonon dispersion of LDA functional at equilibrium lattice constant are close to experimental results while the phonon dispersion of the GGA functional underestimates the experimental results. The theoretical GGA and lattice constant of gold overestimates the frequencies by 7.6% and 4.2%. The analytical calculated phonon dispersions of Ag using IFCs approach of the 1-2NN, 1-5NN and 1-6NN are shown in Figure 4. The red, green and blue line represents the nearest neighbours (NN) respectively. The phonon dispersions of the second neighbour forces (1-2NN) underestimates the experiment at the longitudinal (L) and transverse(T) acoustic branches of the X and L points while at the L and T branches about the W points it is close to experiment. The 1-5NN and 1-6NN phonon dispersion are in good agreement with experimental data. Therefore, in Au the phonons of the IFCs predict well the experimental phonons than those of Quantum Espresso.

5.0 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 Au we observed that the extension to 1 – 6th neighbor gave slightly close agreement with the experimental phonon dispersions results when compared to the 1 – 5th neighbor at W_T and L_L symmetry points. The percentage errors for Au at point W_T are 2.5% and 2.9%, at point L_L we observed 0.6% and 0.7% for 1 – 6th and 1 – 5th neighbours respectively. For Ag, the LDA underestimates the lattice of about 1.6% while the GGA overestimates it by 1.9%. The analytic phonon dispersion curve for Ag also shows that the second neighbour forces (1-2NN) underestimate the experimental except at the longitudinal acoustic branch L about the W point where the frequency is close to experimental results.

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