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Improved Lattice Dynamical Model to Study Phonon Frequencies of Copper in Off-Symmetric Directions

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Abstract *– Our Improved Lattice Dynamical Model based on Generalized Pseudopotential Theory (GPT) is found to be good working in studying lattice dynamics and lattice mechanical properties of transition metals, has been used first time for the theoretical investigation of phonon frequencies of copper in off-symmetric directions. The computed results of phonon frequencies are found to be in good agreement with experimental results with average deviations 12.07 %, 6.51% and 4.76% in* v_1, v_2, *and* v_3 *respectively as well as are also in fairly agreement with other theoretical models. Our model having less number of parameters is found to be capable to reproduce phonon frequencies not only in symmetric but in off-symmetric directions without inclusion of tensor forces and modification.*

Keywords*: Lattice Dynamical Model, transition metal, phonon frequency.*

I. Introduction

The measurement of phonon spectra provide a very direct test of any microscopic theory of lattice dynamics of solids [1], [2].

Transition metals have attracted continuous attention of physicists because of their unusual electronic and structural properties. In transition metals, narrow d-bands are filled and lie below the Fermi energy. This group of metals often exhibit pronounced phonon anomalies as a result of complex fermi-surface geometries in conjunction with strong electron phonon coupling, whose consistent description still provides a challenge for theoretical approaches [3]. Essentially for transition metals, one has to consider the fact that the tightly bound d-electrons hybridize with the nearly free electrons, resulting in a partially filled d-band crossing the fermi energy. The presence of the d-band has been a serious impediment to the application of pseudopotential perturbation theory for such systems.

The ab initio prediction of phonon dispersion of transition and noble metals is a challenging problem that so far has not found a completely satisfactory solution [4]. A paradigmatic example is copper, a noble metal with 3d and 4s valence electrons whose theoretical phonon dispersions have still quite large errors with respect to experiment [2].

It is found that in order to explain fully all static and dynamic properties of noble and transition metals, pseudopotential has to be energy dependent and non-local.

Pseudopotential explains complicated nature of interatomic interactions in metals. Pesudopotential can be used to study higher order terms in the perturbation expansion of energy, which leads to many body forces. In order to study many body forces we have suggested a simple method to generate an effective electron-ion interaction from the energy wave number characteristic

obtained by first principle calculation. This effective potential has been used to study the effect of three-body forces on the lattice dynamics of noble metals by us and we found three-body forces do play important role [5].

During literature survey, we found unlike simple metals, there is not large number of local pesudopotentials used for comprehensive study of physical properties of transition metals. Looking to such requirement, we have carried out extensive studies of the physical properties of transition metals using pseudopotentials [6] - [8].

Any theoretical model can be tested by its capability to reproduce frequencies not only in symmetric but in off-symmetric directions also. In this context, we in the present communication, use our well established lattice dynamical model [6] to study phonon frequencies of copper in off-symmetric directions.

Jani and Gohel [9] used phenomenological model which is successful in symmetric directions but it does not predict phonon frequencies in off-symmetric directions.
Chopra et al [10] used a simple extended de Launay model and obtained much closer agreements for both symmetric and off-symmetric directions.

Luo Ningsheng et al [11] calculated phonon frequencies in symmetric and off-symmetric directions for Cu using the Embedded Atom Method (EAM) without any adjustable parameter, which are in good agreement with experimental results.

The paper is organized as follows. In section – II, we present theory. The computed results are compared with experimental results with necessary discussions in section – III.

II. Theory

Our well established pseudopotential has following form [6].

$$W_i(q) = \frac{1}{\Omega_0}\left[-\frac{8\pi Z}{q^2}\cos q R_c + \frac{\beta}{(1-(qR_d)^2)^4}\right] \qquad (1)$$

Where Z is valency of the metal ion, Ω_0 is atomic volume and R_c is core radius. β is a parameter and R_d is radius of d-electron shell.
Here we have used real space analysis to obtain the vibrational frequencies $\omega_{\vec{q}\lambda}$. For this one essentially requires to diagonalize the dynamical matrix $D_{\alpha\beta}\left(\frac{\rightarrow}{q}\right)$ for different values of qs.
In such analysis interatomic potential which contains pseudopotential is most important ingredient which is used to calculate K_r - radial force constant and K_t - tangential force constant. Finally, dynamical matrix $D_{\alpha\beta}\left(\frac{\rightarrow}{q}\right)$ is calculated using these force constants.

Here it is required to compute $D_{\alpha\beta}\left(\frac{\rightarrow}{q}\right)$ for values of qs in off-symmetric directions. For this purpose, we adopt following method to generate set of q vectors in off-symmetric directions of Brillouin zone for fcc crystal. To generate a set of wave vectors, an irreducible sector of Brillouin zone (1/48 per atom) is defined for fcc lattice by following set of equations [13].

$$(q_x + q_y + q_z) \le \frac{3}{2}$$
$$q_x \le 1$$
$$q_y \le 1$$
$$q_z \le 1 \qquad (2)$$

Dividing the q_x , q_y and q_z axis into z equal intervals

$$q_x = \frac{P_x}{z}$$

$$q_y = \frac{P_y}{z}$$

$$q_z = \frac{P_z}{z}$$

Then we have

$$(P_x + P_y + P_z) \le \frac{3}{2}z \qquad (3)$$

Where P_x, P_y and P_z are integers which are all even or odd.

III. Results and Discussion

The computed values of two force constants and for first few shells are shown in table 1. In table 2 we present our computed phonon frequencies along with experimental results.

TABLE I
THE COMPUTED VALUES OF RADIAL AND TANGENTIAL FORCE CONSTANTS (DYNE/CM) AT TEMRERATURE 0 K FOR FIRST FIVE SHELLS OF COPPER.

Shell No.	T	K_r	K_t
1	0	38956.617188	-3710.051270
2	0	-912.552734	223.261780
3	0	-256.052612	30.404428
4	0	99.849380	29.208412
5	0	-119.678291	25.172459

TABLE II
THE COMPUTED VALUES OF PHONON FREQUINCIES (THZ) FOR COPPER IN OFF-SYMMETRIC DIRECTIONS. THE EXPERIMENTAL RESULTS ARE DUE TO [14] IN THE PARENTHESES. THE UNDERLINED VALUES ARE MEASURED PHONON FREQUENCIES.

10q	v_1	v_2	v_3
0 1 2	1.07(1.35)	1.61(1.89)	2.53(2.80)
0 1 3	1.85(2.15)	2.30(2.60)	3.40(3.85)
0 1 4	2.64(2.95)	3.01(3.25)	4.23(4.75)
0 1 5	3.35(3.60)	3.64(3.84)	5.00(5.50)
0 1 6	3.95(4.12)	4.16(4.33)	5.68(6.20)
0 1 7	4.41(4.54)	4.58(4.74)	6.25(6.70)
0 1 8	4.74(4.85)	4.89(5.03)	6.70(7.05)
0 1 9	4.93(5.06)	5.07(5.17)	7.00(7.20)
0 1 10	4.99(5.14)	5.14(5.25)	7.16(7.30)
0 2 3	1.49(1.92)	2.78(2.93)	4.07(4.48)
0 2 4	2.23(2.62)	3.40(3.54)	4.73(5.15)
0 2 5	3.00(3.38)	3.96(4.14)	5.32(5.80)
0 2 6	3.70(4.00)	4.46(4.53)	5.82(6.32)
0 2 7	4.26(4.42)	4.86(4.90)	6.24(6.72)
0 2 8	4.66(4.77)	5.16(5.19)	6.58(6.97)
0 2 9	4.88(5.00)	5.34(5.33)	6.84(7.08)
0 2 10	4.90(5.07)	5.40(5.36)	7.02(7.10)
0 3 4	2.01(2.56)	3.89(3.95)	5.19(5.60)
0 3 5	2.73(3.17)	4.43(4.44)	5.62(6.04)
0 3 6	3.46(3.85)	4.90(4.81)	5.95(6.37)
0 3 7	4.09(4.32)	5.29(5.13)	6.20(6.69)
0 3 8	4.56(4.70)	5.57(5.40)	6.40(6.81)
0 3 9	4.80(4.91)	5.75(5.55)	6.59(6.80)
0 3 10	4.78(5.00)	5.81(5.61)	6.79(6.81)
0 4 5	2.66(3.17)	4.94(4.77)	5.84(6.27)
0 4 6	3.31(3.75)	5.40(5.15)	6.02(6.48)
0 4 7	3.96(4.23)	5.78(5.47)	6.10(6.62)
0 4 8	4.48(4.62)	6.05(5.67)	6.16(6.64)
0 4 9	4.74(4.86)	6.22(5.81)	6.28(6.55)
0 4 10	4.46(4.93)	6.30(5.90)	6.49(6.50)
0 5 6	3.33(3.80)	5.88(5.50)	6.01(6.59)
0 5 7	3.89(4.24)	5.93(5.80)	6.28(6.57)
0 5 8	4.41(4.58)	5.84(6.01)	6.56(6.45)
0 5 9	4.67(4.84)	5.87(6.15)	6.73(6.26)
0 5 10	4.52(4.88)	6.15(6.18)	6.79(6.18)
0 6 7	3.96(4.23)	5.70(6.14)	6.72(6.37)
0 6 8	4.39(4.60)	5.49(6.16)	7.01(6.35)
0 6 9	4.60(4.84)	5.46(5.97)	7.18(6.46)
0 7 8	4.48(4.66)	5.12(5.88)	7.38(6.68)
0 7 9	4.54(4.90)	5.10(5.70)	7.56(6.76)
0 8 9	4.43(5.02)	4.97(5.47)	7.84(7.06)
1 1 2	0.97(1.45)	1.34(1.68)	3.07(3.28)
1 1 3	1.83(2.18)	2.10(2.40)	3.84(4.13)
1 1 4	2.68(2.94)	2.81(3.05)	4.56(4.92)
1 1 5	3.38(3.65)	3.46(3.69)	5.22(5.68)
1 1 6	3.92(4.15)	4.12(4.29)	5.80(6.30)
1 1 7	4.34(4.59)	4.65(4.73)	6.28(6.75)
1 1 8	4.64(4.87)	5.03(5.07)	6.67(7.02)
1 1 9	4.82(5.03)	5.24(5.25)	6.95(7.22)
1 2 2	1.17(1.52)	1.70(2.15)	3.76(4.05)
1 2 3	1.61(2.06)	2.38(2.74)	4.44(4.69)
1 2 4	2.32(2.65)	3.04(3.30)	5.04(5.39)
1 2 5	3.08(3.43)	3.67(3.91)	5.56(5.92)
1 2 6	3.74(4.03)	4.27(4.43)	5.99(6.42)
1 2 7	4.22(4.41)	4.83(4.86)	6.32(6.77)
1 2 8	4.55(4.75)	5.27(5.19)	6.58(6.98)
1 2 9	4.73(4.94)	5.52(5.43)	6.79(7.07)
1 3 3	1.64(2.15)	2.94(3.23)	5.02(5.27)
1 3 4	2.08(2.58)	3.57(3.78)	5.51(5.76)
1 3 5	2.77(3.24)	4.07(4.26)	5.91(6.18)
1 3 6	3.46(3.86)	4.60(4.68)	6.19(6.59)
1 3 7	4.04(4.29)	5.11(5.11)	6.37(6.84)
1 3 8	4.44(4.62)	5.58(5.39)	6.46(6.95)
1 3 9	4.64(4.81)	5.90(5.63)	6.54(6.90)
1 4 4	2.19(2.79)	4.02(4.12)	5.89(6.20)
1 4 5	2.68(3.20)	4.51(4.53)	6.18(6.48)
1 4 6	3.30(3.74)	4.96(4.97)	6.37(6.69)
1 4 7	3.91(4.23)	5.37(5.34)	6.45(6.80)
1 4 8	4.36(4.56)	5.77(5.62)	6.44(6.75)
1 4 9	4.57(5.75)	6.17(5.83)	6.38(6.58)
1 5 5	2.86(3.37)	4.92(4.90)	6.38(6.68)
1 5 6	3.31(3.80)	5.26(5.28)	6.52(6.73)
1 5 7	3.84(4.21)	5.49(5.63)	6.62(6.71)
1 5 8	4.31(4.55)	5.64(5.87)	6.70(6.63)
1 5 9	4.52(4.75)	5.81(6.05)	6.78(6.40)
1 6 6	3.54(3.87)	5.42(5.57)	6.68(6.70)
1 6 7	3.92(4.23)	5.42(5.84)	6.87(6.67)

1 6 8	4.31(4.55)	5.35(5.91)	7.05(6.62)
1 7 7	4.14(4.38)	5.23(5.86)	7.14(6.66)
1 7 8	4.42(4.61)	5.00(5.72)	7.36(6.78)
1 8 8	4.61(4.77)	4.66(5.55)	7.61(6.99)
2 2 3	1.76(2.27)	2.10(2.42)	5.02(5.20)
2 2 4	2.40(2.84)	2.70(3.00)	5.54(5.80)
2 2 5	3.18(3.52)	3.29(3.54)	5.99(6.25)
2 2 6	3.70(4.04)	4.07(4.24)	6.28(6.60)
2 2 7	4.08(4.38)	4.83(4.88)	6.47(6.81)
2 2 8	4.36(4.66)	5.47(5.32)	6.56(6.96)
2 3 3	1.91(2.38)	2.37(2.86)	5.56(5.72)
2 3 4	2.26(2.80)	2.91(3.31)	6.01(6.18)
2 3 5	2.88(3.35)	3.48(3.80)	6.35(6.50)
2 3 6	3.45(3.80)	4.12(4.36)	6.56(6.78)
2 3 7	3.91(4.21)	4.84(4.94)	6.64(6.89)
2 3 8	4.20(4.47)	5.54(5.40)	6.58(6.93)
2 4 4	2.32(2.89)	3.36(3.73)	6.38(6.55)
2 4 5	2.72(3.27)	3.84(4.11)	6.64(6.77)
2 4 6	3.27(3.72)	4.33(4.55)	6.78(6.92)
2 4 7	3.75(4.17)	4.90(5.04)	6.86(7.02)
2 4 8	4.07(4.41)	5.52(5.51)	6.76(6.91)
2 5 5	2.86(3.41)	4.20(4.43)	6.83(6.96)
2 5 6	3.25(3.73)	4.55(4.78)	6.93(7.03)
2 5 7	3.70(4.10)	4.91(5.16)	6.93(7.01)
2 5 8	4.04(4.38)	5.30(5.52)	6.88(6.85)
2 6 6	3.46(3.90)	4.74(4.99)	7.02(7.06)
2 6 7	3.80(4.18)	4.90(5.24)	7.06(7.01)
2 7 7	4.00(4.29)	4.80(5.36)	7.17(6.94)
3 3 4	2.40(2.98)	2.60(3.03)	6.45(6.63)
3 3 5	2.93(3.44)	3.08(3.46)	6.73(6.88)
3 3 6	3.37(3.81)	3.82(4.08)	6.87(7.05)
3 3 7	3.68(4.09)	4.64(4.76)	6.87(7.08)
3 4 4	2.49(3.05)	2.77(3.32)	6.79(6.94)
3 4 5	2.80(3.34)	3.18(3.70)	7.01(7.07)
3 4 6	3.20(3.69)	3.75(4.15)	7.09(7.13)
3 4 7	3.50(3.95)	4.47(4.70)	7.04(7.12)
3 5 5	2.84(3.46)	3.47(3.96)	7.16(7.20)
3 5 6	3.14(3.68)	3.84(4.20)	7.20(7.18)
3 5 7	3.44(3.99)	4.35(4.60)	7.13(7.15)
3 6 6	3.31(3.78)	4.00(4.44)	7.22(7.22)
4 4 5	2.72(3.40)	2.89(3.43)	7.25(7.26)
4 4 6	3.00(3.62)	3.44(3.86)	7.27(7.31)
4 5 5	2.82(3.43)	2.88(3.54)	7.36(7.34)
4 5 6	2.95(3.55)	3.28(3.80)	7.33(7.30)

Our results are excellent with 12.07 %, 6.51% and 4.76% deviations in ν_1, ν_2 and ν_3 respectively with experimental values. Our results are better than results of Jani and Gohel [9] and Chopra and Laziz [10] while it is also well compared with theoretical results of Luo Ningshen et al [11]. It is interesting to note here that these authors have also found that phonon frequencies in symmetric and off-symmetric directions are good. We also find that our model is also generating phonon frequencies in symmetric and off-symmetric directions equally well. Luo Ningshen et al [12] used Embedded Atom Method (EAM) and found that EAM cannot assure to reproduce the phonon frequencies at zone boundaries for Cu, Ni and Pd. In order to reproduce the measured phonon frequencies accurately they provide a method with the modification of the force field of the third neighbor potentials by considering somewhat non uniform distribution of electron in real transition metals. Our results are better in the sense that we have not used such fitting procedure. Here we also like to mention that the present pseudopotential has been used for study of lattice dynamics of large number of transition metals (empty d-band, filled d-band, partially filled d-band) using same philosophy [6]. For further test of our pseudopotential and computed phonon frequencies in off-symmetric directions, large number of lattice mechanical properties like Debye Waller factor, mean square displacement, thermal expansion, Debye temperature, specific heat, Gurunesian parameter are computed for many transition metals with good degree of success [6], [13]. No such attempt has been done in past for reliability of the computed phonon frequencies in off-symmetric directions. At last we like to comment that we have not used any tensor force constant or any angular force and our model has less number of parameters. It is in this context our results should be regarded more satisfactory in comparison with all available theoretical results.

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