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Lattice Dynamics of Face Centred Cubic Crystals

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Authors' contributions

This work was carried out in collaboration between both authors. Author YAS performed the statistical analysis and wrote the first draft of the manuscript. Author GB designed the study and managed the analyses of the study. Author YAS managed the literature searches. Both authors read and approved the final manuscript.

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Original Research Article

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ABSTRACT

Lattice dynamics of fcc metal crystals have been studied within the harmonic approximation. Phonon dispersion relation (frequency as a function of wave vector) along the symmetry directions [100], [110] and [111], density of states and the heat capacity have been calculated for Aluminum, Copper and Lead using lattice dynamics model *debye*. The results obtained were compared with results from neutron scattering experiment. The calculated results of phonon dispersion relations as well as the heat capacities are generally in good agreement with the experimental results.

Keywords: Lattice dynamic; density of states; dispersion relation; harmonic approximation; heat capacity.

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1. INTRODUCTION

Many properties of solids materials depend on the dynamics of the crystal lattice which is the motion of atoms about their equilibrium positions. The motion of atoms in metallic crystals is essentially a many body problem of a several electrons interacting with the ions that constitute the lattice [1]. Lattice dynamical properties play a vital role in the advancement of solid state physics. Several experimental techniques such as inelastic neutron scattering [2,3] and x-ray diffraction [4] for investigating the lattice dynamics of materials have been developed. Attempts have also been made by physicist to calculate the lattice dynamic properties theoretically using model simulations and quantum mechanical calculations [5].

K. Mohammed et al. [6] used the ionic Morse potential immersed in a sea of free-electron gas to study lattice vibrations in six face-centered-cubic metals (i.e., copper, silver, gold, lead, palladium, and nickel) by computing phonon dispersion relations along the principal symmetry directions, and the Debye temperature, the mean-square displacement, the effective x-ray characteristic temperature, and the Debye-waller factor exponent, as a function of absolute temperature (T). The computed results are in excellent agreement with the available experimental observations for almost all the metals studied. Xu et.al calculated the phonon dispersion in Copper by developeing a new method of mapping phonon dispersion relations using momentum-resolved x-ray calorimetry in which X-ray scattering intensities were measured at selected points in reciprocal space. They extracted the thermal part of the scattering intensity by scanning the temperature of the sample and analyzed the intensity variations to yield the energies of the phonons [7]. Their results were in excellent agreement with the known phonon dispersion relations. A computer program PHON was also used to calculate the Phonon dispersion relations for Aluminum using 4 x 4 x 4 and 8 x 8 x 8 super cell and equispaced grid of q-points [8]. The original model of Sarkar et al. for cubic metals in extending the ion-ion interaction, ion-electron interaction and the introduction of crystal equilibrium condition was modified by Coelho and Shukla [9]. They calculated the phonon dispersion relations along the three principal symmetry directions and the thermal properties of copper, silver and gold and they obtain good results which are in agreement with the experimental findings. Born–von K´arm´an theory of lattice dynamics and the modified analytic embedded atom method were employed by Jun to reproduce experimental results of the phonon dispersion in copper at zero pressure along three high symmetry directions and four off-symmetry directions [10]. The results show that the shapes of dispersion curves at high pressures are very similar to that at zero pressure. Direct method and ab initio force constants [11] and density functional perturbation theory DFPT implemented in ABINIT code using first principles [12] were also used to calculate the lattice dynamical properties in fcc crystal. Most of the results obtained are in good agreement with the experimental data. Phonon dispersion relation and density of states for Al and Cu were calculated using a theoretical model *debye* by Yusra et al. [13].

In this paper lattice dynamics of Al, Cu and Pb have been studied within harmonic approximation using a theoretical model debye.

2. METHODOLOGY

The lattice dynamics model of this paper is based on a harmonic interaction with one free parameter, the force constant of the nearest neighbor interaction. The starting point is an fcc crystal in which every atom oscillate about its equilibrium position. Given a harmonic interatomic potential, we then find a plane wave harmonic solutions to the equation of motion of the atoms.

The total harmonic potential of a three-dimentional crystal can be written [14] in terms of the displacement vector, **u** of each atom from its equilibrium position, **R** as

$$U^{harm} = \frac{1}{2}\sum_{\boldsymbol{R}\boldsymbol{R}'} u(\boldsymbol{R}).D(\boldsymbol{R}-\boldsymbol{R}').\mathrm{u}(\boldsymbol{R}') \qquad (1)$$

where the sum extends over all pairs of atoms located at **R** and $\mathbf{R}'$. Force as a function of the potential is given as,

$$F = -\nabla U^{harm} = -\frac{\partial U^{harm}}{\partial u(\boldsymbol{R})} \qquad (2)$$

From Newton's second law of motion, force is given as,

$$F = Ma = M\ddot{u}(\boldsymbol{R}) \qquad (3)$$

The motion of atom of mass M can be obtained from equations 2 and 3,

$$\text{M}\ddot{u}(\boldsymbol{R}) = -\sum_{R'} \ddot{D}(\boldsymbol{R}-\boldsymbol{R}').u(\boldsymbol{R}'). \quad (4)$$

The above equation has a solution of the form,

$$\text{u}(\mathbf{R},\text{t})= \epsilon_p e^{i[\boldsymbol{q}.\boldsymbol{R}-\omega_P(\boldsymbol{q})t]} \quad (5)$$

where p (p=1,2,3) is one of the three polarization vectors and ω_p (**q**) is the phonon frequency associated with polarization p and wave vector **q** determined from the dynamical matrix

$$\text{D}(\mathbf{q}) = \sum_{\mathbf{R}} \text{D}(\mathbf{R})\text{e}^{-\mathbf{iq}.\mathbf{R}} \quad (6)$$

The three polarization vectors ϵ_p are the real eigen vectors of the dynamical matrix and the angular frequency $\omega_p(\boldsymbol{q})$ is given in terms of the corresponding eigen value, λ_p as

$$\omega_p(\boldsymbol{q}) = \sqrt{\lambda_p(\boldsymbol{q})/M} \quad (7)$$

If we assume that the interatomic pair potential, *Φ* contributes to the sum in equation (1) only for nearest neighbors then equation (4) reduces to a sum over 12 nearest neighbors **R** in an fcc crystal,

$$D(\boldsymbol{q}) = Bsin^2(\frac{1}{2}q.\boldsymbol{R})\hat{\mathbf{R}}\hat{\mathbf{R}} \quad (8)$$

where $\hat{R}\hat{R}$ is the dyadic (the outer product) $(\hat{\mathbf{R}}\hat{\mathbf{R}})_{ij} = \hat{\mathbf{R}}_i\hat{\mathbf{R}}_j$ of the unit vectors $\hat{\mathbf{R}}=\mathbf{R}/R$. The force parameter B is given as B = 2 *Φ*"(d), where d is the equilibrium nearest neighbor distance.

A simple Monte is then used to obtain the phonon density of states, g(ω), by calculating the number of phonon frequency N(ω) in the frequency interval ω to ω + ∇ω in the first brillouin zone, determine the dynamical matrix D in Eq.6 for each of the sampled wave vectors **q**, and then compute the three phonon frequencies ω_p (**q**) from the three eigen values according to Eq.5. N(ω) is then used to calculated the density of state using

$$\text{g}(\omega) = \frac{\text{N}(\omega)}{\text{N}_{\text{MC}}\boldsymbol{\Delta\omega}}\frac{4}{\text{a}^3}\text{V} \quad (9)$$

where *a* is the lattice constant of the crystal with atomic density, *n = N/V.*

The thermal contribution to the internal energy per unit frequency interval of a crystal is then calculated using

$$\text{U}(\omega,T) = g(\omega)\varepsilon_T(\omega,T) = g(\omega)\hbar\omega\frac{1}{e^{\hbar\omega/kT}-1} \quad (10)$$

Where $\varepsilon_T(\omega,T)$ is obtained from the average energy associated with a normal mode of frequency ω in equilibrium with a heat bath of temperature, T given by;

$$\varepsilon(\omega,T) = \hbar\omega(\frac{1}{e^{\hbar\omega/k_BT-1}} + \frac{1}{2}) \equiv \varepsilon_T(\omega,T) + \frac{1}{2}\hbar\omega \quad (11)$$

The total thermal energy of a crystal is the integral (or sum) over all frequencies ω of the internal energy density *U(ω,T)*

$$U(T) = \int_0^\infty d\omega U(\omega,T) \quad (12)$$

The heat capacity per unit volume $C_v$then follows from the temperature derivative of the internal energy U(T).

$$\boldsymbol{C_V(T)} = \frac{\boldsymbol{1}}{\boldsymbol{V}}\frac{\boldsymbol{\partial}}{\boldsymbol{\partial T}}\int \boldsymbol{d\omega}\, g(\omega)\frac{\hbar\omega}{e^{\hbar\omega/kT}-1} \quad (13)$$

3. RESULTS AND DISCUSSION

Based on the semi classical theory of lattice dynamics, the dispersion relations along three high symmetry direction and heat capacities for three fcc metals Al, Cu and Pb were calculated using numerical simulation.

Figs. 1, 2 and 3 shows the phonon dispersion curves along high symmetry directions [100], [110] and [111] for Al, Cu and Pd respectively. Blue points represent the calculated results while green, orange and black represents experimental results from neutron scattering for comparison. The notations *X, K* and *L* represent symmetry points on the surface of the first Brillouin zone. It can be observed that the simulated phonon dispersion curves for the fcc metals are generally in good agreement with the available experiment results but the agreements are better in case of Al and Cu. The phonon dispersion curves reproduced very well the experimental results along high symmetry directions especially near lower frequency. In the high-frequency limit, it can be seen that there is a slight deviation from the experimental results. The deviations of the simulation results from experimental results appear more in Pb especially between the frequency range of $5\times10^{12}rad/s$ to $15\times10^{12}rad/s$ and $20\times10^{12}rad/s$ to $40\times10^{12}rad/s$ in Al. This may be as a result of the simulation done within harmonic approximation with only one adjustable parameter.

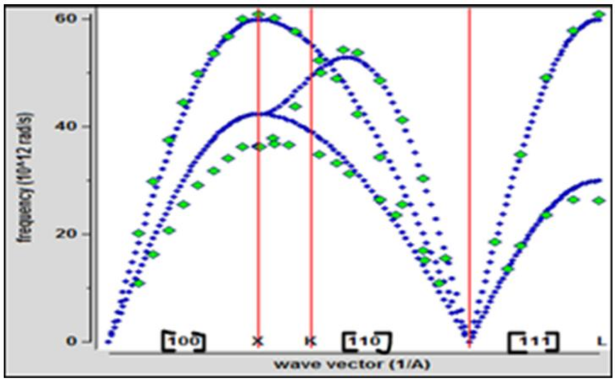

Fig. 1. Phonon dispersion relation in Al. Blue points represents present calculation, green represent experimental points

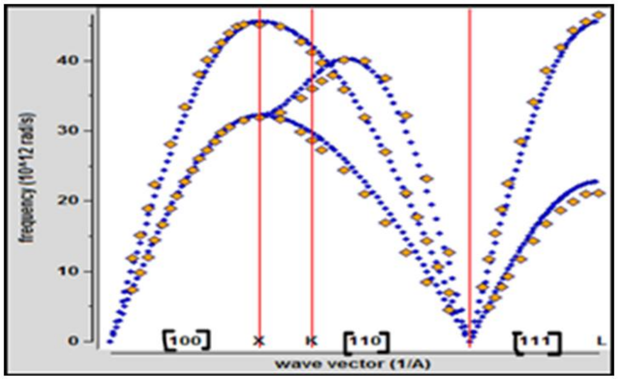

Fig. 2. Phonon dispersion relation in Cu. Blue points represents present calculation, orange represent experimental points

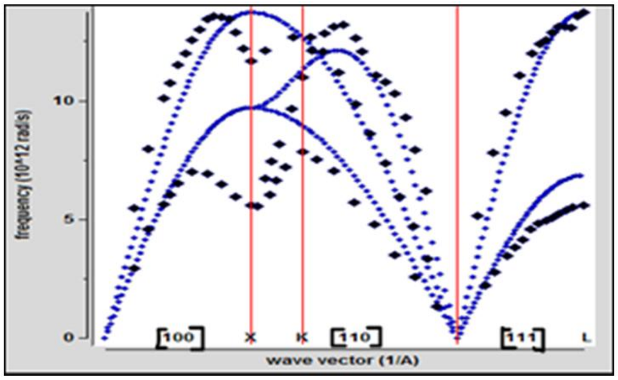

Fig. 3. Phonon dispersion relation in Pb. Blue dots represent simulation, black represent experimental result

The density of states for the crystals is obtained using the dispersion relation. The calculated density of states function, normalized to $\int_0^\infty \mathrm{d}\omega g(\omega) = 3\mathrm{N}$, (where 3N is the number of phonon modes in a crystal with N atoms) as shown Figs. 4, 5 and 6.

Figs. 4, 5 and 6 represent the density of states for Al, Cu and Pb respectively. The peaks in the density of states correspond to the high phonon density regions of the dispersion curve. The density of states is high in the regions where dispersion curve is flat. The derivative of density of states with respect to frequency has a singularity at frequencies in which the dispersion relation has a horizontal tangent.

Figs. 7, 8 and 9 compared the predicted heat capacity from the *debye* lattice dynamics simulation, the Debye model and heat capacity from neutron scattering experiment for Al, Cu and Pb respectively. It is observed from the figures that simulated heat capacity for all the three metals Al, Cu and Pb are in good agreement with heat capacity from neutron scattering experimental as well as the heat capacity obtained from Debye model.

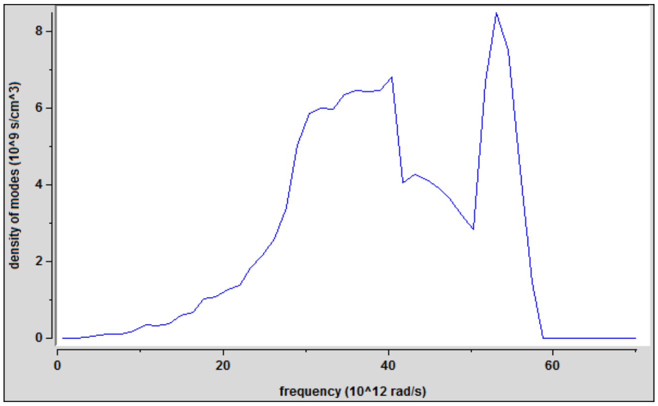

Fig. 4. The calculated phonon density of states in Al

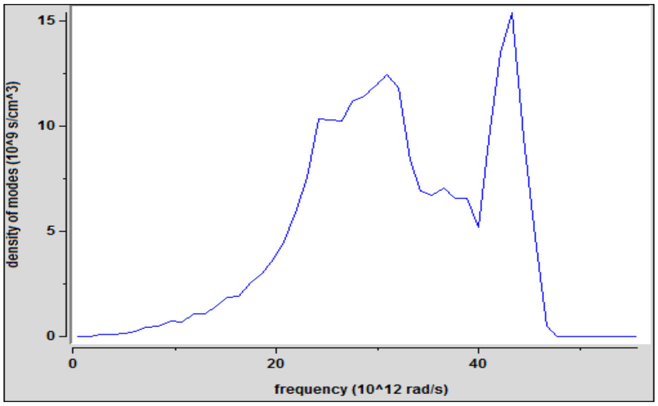

Fig. 5. The calculated phonon density of states in Cu

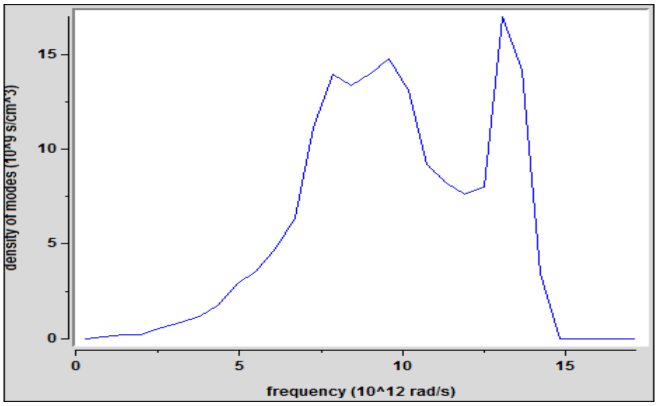

Fig. 6. The calculated phonon density of states in Pb

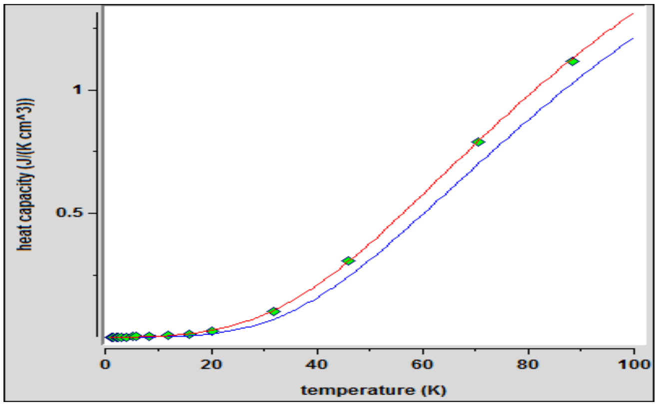

Fig. 7. Heat capacity of Al. Numerical simulation in blue, the Debye model in red and the point represent neutron scattering experimental result

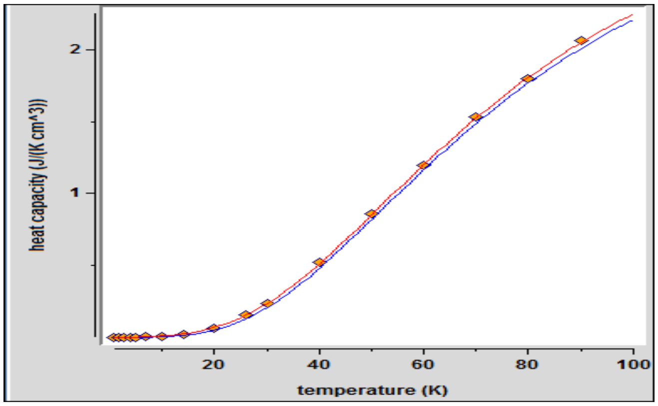

Fig. 8. Heat capacity of Cu. Numerical simulation in blue, the Debye model in red and the point represent neutron scattering experimental result

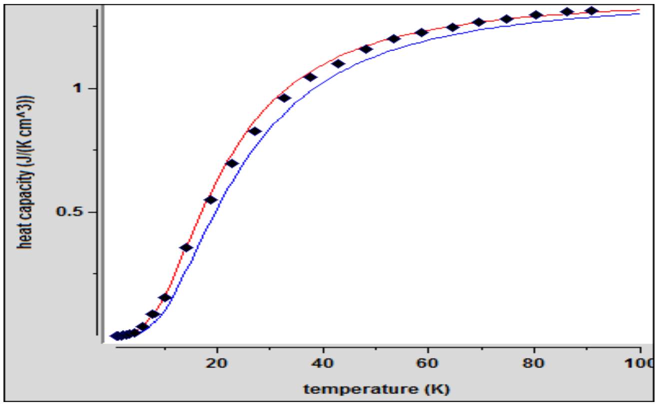

Fig. 9. Heat capacity of Pb. Numerical simulation in blue, the Debye model in red and the point represent neutron scattering experimental result

4. CONCLUSION

Lattice dynamical properties lay a foundation for studying specific heat, thermal expansion, thermal conductivity, phase transitions, sound propagation and electron phonon interaction of solid materials. In this paper, Phonon dispersion relation, density of states and heat capacity in Al, Cu and Pb have been calculated using a theoretical model *debye.* The results obtained were compared with experimental results from neutron scattering. The phonon dispersion curves along high symmetry directions [100], [110] and [111] are in good agreement with the experimental results especially at lower frequencies. The calculated heat capacities for all the three metals are also in good agreement with experimental findings.

There is only one ajustable parameter in the model used, yet it gives an excellent agreement between the calculated and the experimental results for phonon dispersion relations, as well as the heat capacity of all the metals studied. The success of a lattice-dynamical model is judged by its ability to reproduce the experimental phonon. This paper presents a successful test to the validity of the theoretical model *debye* and possibility of using the model in calculation and analysis of other lattice dynamics properties.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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