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Phonon Dispersion Curves Of Some Transition Metals

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Abstract

This study presents a comprehensive investigation of the phonon dispersion curves of some transition metals, including titanium (Ti), vanadium (V), chromium (Cr), manganese (Mn), iron (Fe), cobalt (Co), nickel (Ni), copper (Cu), and zinc (Zn). Using density functional theory (DFT) and the linear response method, we calculated the phonon dispersion curves and phonon density of states (PDOS) for these metals.

Keywords: Phonon dispersion curves, transition metals, density functional theory, linear response method, phonon density of states

INTRODUCTION

In transition metals the unionised free atoms contains an incomplete shell of lower principal quantum number than the outer shell. The d -electrons in the transition metals are not sufficiently localised and mixing of d and s electronic states give rise to allotrophy and multiple chemical valencies and creates complications in the theoretical studies. Here results obtained by the present theoretical calculations on three transition metals palladium, thorium and nickel have been discussed. All the three transition metals have FCC structure. d-band electronsin transition metals have been treated as rigidly bound with the core of the atom.

TABLE –(1) Input data for the determination of model parameters of metals.

Elements	Elastic constants $\times 10^{11}$ dynes cm^2	Ref. For Elastic constants	Phonon frequencies in Hz.	Ref. For Phonon
	C_{11} C_{12} C_{44}		L_0 T_0	
Palladium	22.700 17.590 7.170	[1]	6.700 4.500	[4]
Thorium	7.530 4.890 4.780	[2]	3.474 2.259	[5]
Nickel	24.600 15.000 12.200	[3]	8.560 6.270	[6]

TABLE –(2) Values of physical quantities used in the calculations.

Elements	Atomic radius $x10^{-8}$cm	Lattice constant $x10^{-8}$cm	Atomic mass $x10^{-24}$cm	F.S. Wave vector K_F $\times 10^8$cm	Screening multiplication constant σ
Palladium	1.2071	1.945	176.624	0.898	0.6369
Thorium	1.5785	2.542	385.183	1.532	0.8322
Nickel	1.0937	1.762	97.458	1.175	0.1290

TABLE –(3) Values of model parameters and electron bulk-modulus of transition metals.

Elements	Force constants P Q $a_1 a_2$	Bulk-Modulus K_e $\times 10^{11}$dynes cm^{-2}
Palladium	-0.29945 0.19240 35.35948 2.04857	1.00
Thorium	-0.243297-0.002522.7755-1.5122	0.52
Nickel	-0.38658-0.068468.00642-2.09969	7.40

PALLADIUM

It possesses complex Fermi surface and strong s-d hybridization. Long range interatomic forces are also believed to exist in this metal. Consequently, crystal- dynamics of palladium has not been studied extensively In the past by theoreticians or experimental workers. Exhaustive experimental measurements of phonon dispersion relations for palladium have been made by Miller and Brockhouse at 120°k, 296°k, 673°k and 853°k using inelastic scattering of neutrons.

Earlier efforts of Lahteankorva[49] and Brown[50] for. Studying the lattice dynamics of palladium received partial success. In recent years a number of theoretical workers made lattice dynamical calculations for palladium on the basis of phenomenological models and model potential or pseudopotential approach.

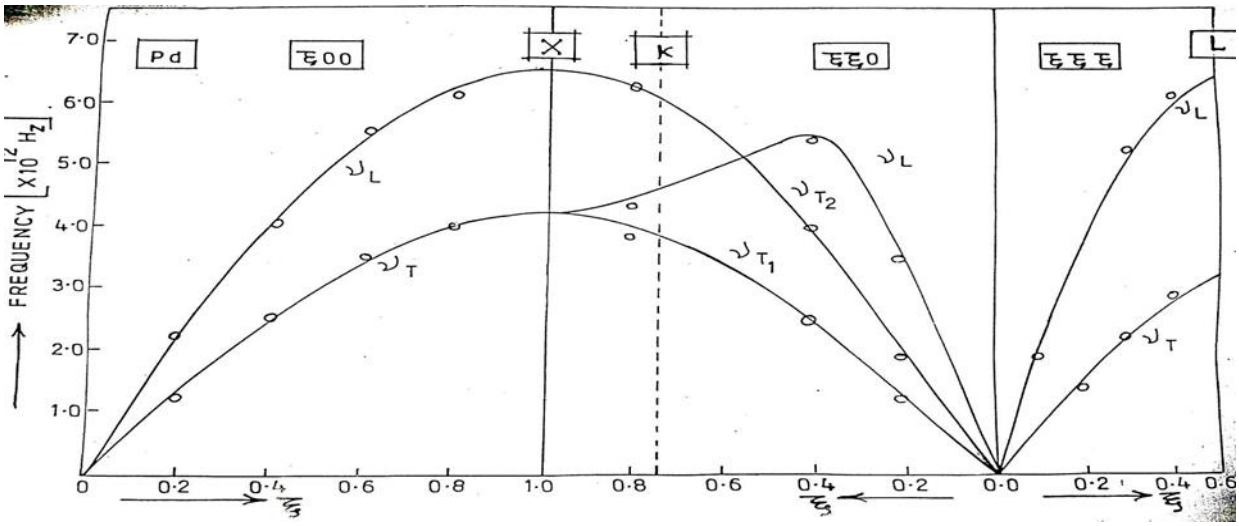

fig.(1):- Phonon dispersion curves for palladium along symmetry directions. Experimental points (0) are due to miller and brockhouse.

Prakash and Hemker[51], Goel et al[52] and Bertolo and Shukla[53] used deLaunay and C.G.W. type angular force, modified Sharma and Joshi model and modified version of Bhatia model respectively to compute the phonon-frequencies ofpalladium along symmetry directions. S. Pal[54] studied the lattice dynamics of palladium applying Cheveaumodeel[55]. Closs and Shukla exploited the axially symmetric model in conjunction with Krebs approach for ion-electron interactions.

Rathore[56] has computed phonon dispersion relation of palladium using a non-central force model including Cheveau scheme for ion-electron interactions and have claimed good agreement with the experimental data. Recently Thakur and Singh[7] have applied a three body phenomenological model to analyse the phonon dispersion curves for transition metals including palladium.

We have compared our phonon dispersion relations for palladium with experimental data of Miller and Brockhouse[15] (at 296°k) in (Fig.1). It is obvious from the graph that our calculated results are in good agreement with the experimental results for all branches except for T mode along [] direction.

THORIUM

Thorium is the second member of actimide series of rare earth metals. Transition metals possessing the outer electronic configuration $7s^26d^2$outside a randon core, 6d and 7s level, hybridize to form a conduction band similar to that of transition metals and 5f shell are empty but located not too far above the Fermi-level. It is believed that 5f levels of thorium possess itinervant character and its hybridization with conduction bands may be appreciable.

Although the energy bands of thorium near Fermi-level do have d-like character, the number of occupied d-states is relatively small compared to those in noble metals or nickel. However, since there are a large number of d-like states just above the Fermi-level in thorium its excitations induced by electron phonon interaction which is expanded to be large because of thorium being super conductor, cause the electrons to spend a part of their time in specially extended d-electron like states.

The phonon frequencies along symmetry directions for thorium are plotted in (Fig.2) below. Experimental points due to reese et al are given for comparison. It is observed the calculated curves compare quite well with the experimental curves except a very small deviation in longitudinal mode along [ξξξ] direction, our results compare well with those of Thakur and Singh[7] for this metal. In an earlier study Resse et al[57] made an attempt to explain their experimental results taking interactions upto seventh neighbour with a large number of twenty four parameters.

Rathore and Verma[58] used a five parameter angular force electron gas model for lattice dynamical study of thorium. Bertolo and Shukla[53] applied modified Bhatia model and model of Lehman et at[59] respectively for calculating phonon dispersion relations of thorium. Gupta et al[60] used a model that assumes short range pair-wise forces effective upto second nearest neighbours and ion-electron interaction on the line of Bhatia for studying lattice dynamics of thorium.

Awasthi and Kushwaha[61] calculated the phonon frequencies and specific heats of thorium using a model that considers interactions between ions in terms of two body (central) and three body(unpaired) forces and evaluates the effect of electron-ion interaction through a screened Coulomb potential.

Rosengren et al[62], J. Kumar[63] and Vrati et al[64] proposed and used some other forms of model potential for the purpose of studying lattice dynamics of thorium. Almost all the attempts received moderate success which might be expected owing to their limitations and short-commings in their approaches.

Comparison of our results with that reported by recent workers[7,58,60,63] shows that our results are in better agreement with the experimental data on phonon dispersion relation of thorium.

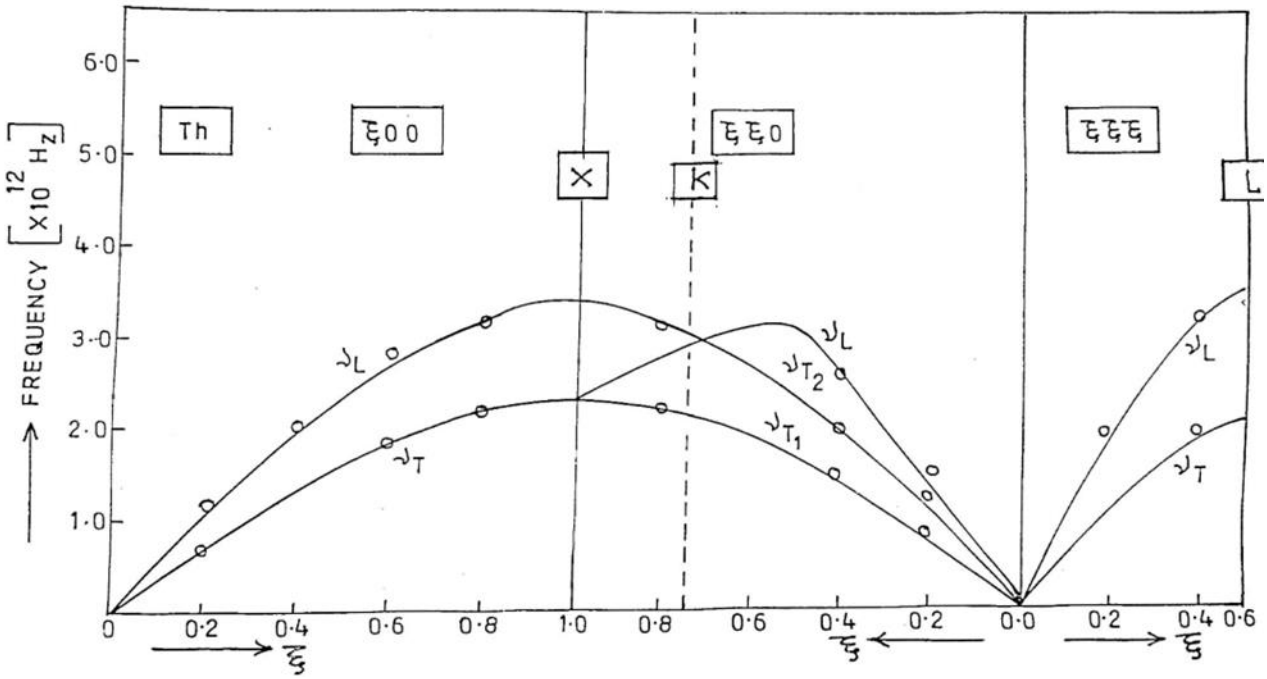

Fig.(2):- Phonon dispersion curves for thorium along symmetry directions. Experimental points (0) are due to reeseet al.

NICKEL

Nickel belongs to the Ferro-magnetic 3d-transition group. The incomplete d-electronic shell is believed to made an important contribution to its very large cohesive energies and its effect on the dispersion relation is also large.

A striking feature presented by this metal is that it display similarity in the properties with some of the metals belonging to two different groups of periodic table. The incomplete shell and its Ferro-magnetic character exhibit its resemblance with iron and cobalt, whereas its electronic structure and Fermi-surface are similar to those of copper in some respects.

Earlier, several theoretical workers reported their calculations on phonon dispersion relations of nickel using phenomenological models. Singh and Prasad[65] evaluated the phonon dispersion relations for nickel on the basis of three phenomenological models. Applying modified Bhatia model the phonon dispersion curves and frequency distribution function of nickel have been studied by Bertolo and Shukla[53].

Closs and Shukla[59] exploited a model in which an axially symmetric ion-ion interaction has been added to the ion- electron interactions term from Krebs approach, for the purposes, They claimed a good agreement between computed and experimental results.

S. Pal's calculations of lattice dynamical properties of nickel, based on deLaunay model have shown reasonable agreement with the experimental observations. Kumar and Hemker[18] calculated the dispersion relations of nickel using pairwise forces for short-range and Kreb's approach for long-range Coulomb forces. Very recently, Kharoo et al[66] also studied the lattice vibration of nickel taking angular interaction on the line of the Clark, Gazis and Wallis[67] approach and volume forces on the Kreb'sscheme[78]. With the claim of better agreementwith the experimental observations in comparison to some previous calculations.

The phonon dispersion curves of nickel as obtained on the basis of the present theoretical formulation are shown in (Fig.3). The experimental results given by Birgeneau et al[67] have also been plotted for comparison. Present results is in good agreement with the experimental one.

Birgeneau[67] obtained his experimental results at room temperature by coherent inelastic scattering of neutrons. Also Dewit and Brockhouse[68] obtained the phonon dispersion relations of nickel along high symmetry directions at room temperature using coherent inelastic scattering of neutrons.

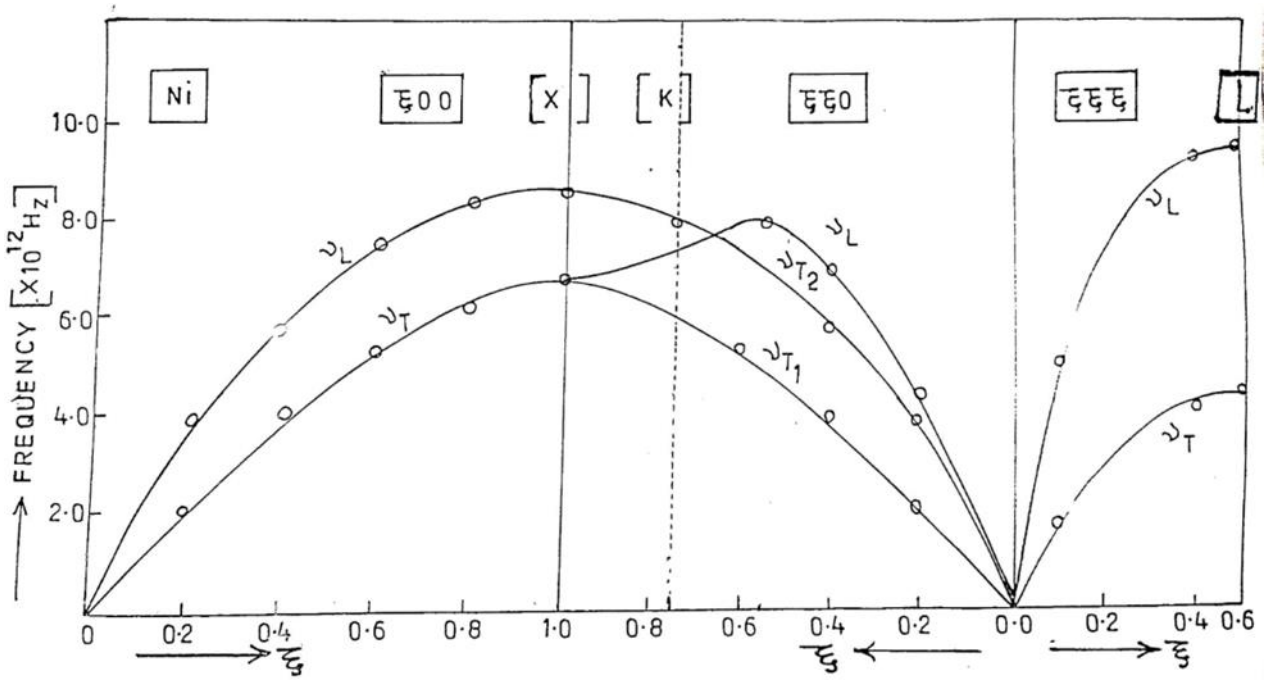

Fig.(3):- Phonon dispersion curves for nickel along symmetry directions. Experimental points (o) are due to Birgeneau et al.

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