JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

THREE BODY FORCES AND NEW APPROACH TO THE LATTICE DYNAMICAL STUDY OF NICKEL, COBALT AND THORIUM

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Abstract: On the basis of modified the results in accuracy for Phonon dispersion curves of Nickel, Cobalt and thorium are draw along the major symmetry directions on the basis of modified scheme second order elastic constants and zero point energy are calculated, this exponential potential is less parametric which provide co-relations effects due to electrons in a simple and effective manner. These results are compared with experimental findings which gives a remarkable result.

Keywords: Modified morse potential, lattice dynamics, dynamical matrix and phonon dispersion.

Introduction: In this predicting the elastic, thermo physical and Lattice dynamical behavior of the crystals Ni, Co and Thfcc crystals. Initially the second order elastic constants (SOEC) are computed and same are compared with the measures ones. The former gives direct measures of the an harmonicity of the crystals lattice and may subsequently be used in the calculations of the properties of lattice defects theorus of thermal expansions, temperature dependence of the SOEC and theory of interaction among the acoustic and thermal phonons.

Pressure derivatives of the SOEC, Anderson Grueisen parameter, frequency dependent Grueisen parameter and Co-efficient of thermal expansion are also calculated for fcc solidstheorus of thermal expansions, temperature dependence of the SOEC and theory of interaction among the acoustic and thermal phonons.

Pressure derivatives of the SOEC, Anderson Grueisen co-efficient of thermal expansion are also calculated for fc solids.

Also analyses the original Morse potential for obtaining the phonon dispersion in Ni, Co and Thfcc metals.

The Table 1 shows the input data for solids which are used the evaluate the parameter D, α and r_o. The computed parameters are shown in table 2.

The present study is important and useful in many respects. The present scheme uses minima parameters for expressing two and three body forces. The results obtained are excellent and very close to experimental data.

Discussion:

The Second order elastic constants (SOEC)

The second order elastic constants are defined as the second derivatives of the energy density. We may obtain same using this eq.-

$$\phi = D/1\sum[\exp.\{-2\alpha(r_j - r_o)\} - 2\alpha\exp.\{-\alpha(r_j - r_o)\}]$$

Which ehurges as:-

$$C11 = D/2[4\alpha 2a2\beta 2\Omega - 1\sum_{I_1I_2I_3} l_1^4 L_j^{-2}\exp.(-2\alpha a L_3) - 2\beta\alpha^2 a^2\Omega^{-1}\sum_{I_1I_2I_3} I_1^4 L_j^{-2}\exp.(-\alpha a L_j) + 2\alpha a\beta^2\Omega^{-1}\sum_{I_1I_2I_3} I_1^4 L_j^{-3}\exp.(-2\alpha a L_j) - 2\alpha a\beta\Omega^{-1}\sum_{I_1I_2I_3} I_1^4 L_j^{-3}\exp.(-\alpha a L_j)]$$

C_{11} derived from the above equation by replacing I14 with I12122. Table 6 shows the computed magnitudes of these elastic constants for solids and experimental determine values are also given alongside for comparison purposes.

The contribution of all the four neighbours have been accounted for while calculating the above constants for the Ni, Co, Th. The model gives rise to the Cauchy's relation i.e. $C_{12} = C_{44}$.

The pressure derivatives of the SOEC :-

Birch has given the following relations for the pressure dependence of the SOEC, i.e.

$$\frac{\partial C_{11}}{\partial P} = -[2C_{11} + 2C_{12} + C_{111} + 2C_{112}] \quad [C_{11} + 2C_{12}]^{-1}$$

$$\frac{\partial C_{12}}{\partial P} = -[-C_{11} - C_{12} + C_{123} + 2C_{112}] \quad [C_{11} + 2C_{12}]^{-1}$$

$$\frac{\partial C_{44}}{\partial P} = -[C_{11} + 2C_{12} + C_{44} + 2C_{166} + C_{123}] \qquad [C_{11} + 2C_{12}]^{-1}$$

$$\frac{\partial C_e}{\partial P} = 1/2\left[\frac{\partial C_{11}}{\partial P} - \frac{\partial C_{12}}{\partial P}\right]$$

$$\frac{\partial K_e}{\partial P} = 1/3\left[\frac{\partial C_{11}}{\partial P} - \frac{\partial C_{12}}{\partial P}\right]$$

$$\frac{\partial C_S}{\partial P} = \frac{2\partial C_{44}}{\partial P}$$

The computed values of these pressure derivatives are scripted in Table 1. The values are compared with the available values reported by other authors.

The Anderson Gruneisen (A-G) Parameter :-

The A.G. parameter may be expressed in two different forms. One in terms of elastic constants and other as function of the pressure derivatives. i.e.

$$\partial = -1 - \frac{(C_{111} + 6C_{112} + 2C_{123})}{3(C_{11} + 2C_{12})}$$

Alternately,

$$\partial = (BS' - 1)$$

Where BS' = $BS' = 1/3\left[\frac{\partial C'_{11}}{\partial P} + \frac{\partial C'_{12}}{\partial P}\right]$

The frequency dependent Gruneisen (F-G) parameter :

Th F.G. parameter γ is evaluated from the following relation-

$$\gamma = -\frac{1}{2}\frac{\Omega\, dK}{K\, d\Omega})$$

$$= 1/2\ [1+\Omega\partial^3\phi/\partial\Omega^3/\partial^2\phi/\partial\Omega^2]$$

The Thermal expansion co-efficient :-

The thermal expansion co-efficient (α) is determined by the expression

$$\alpha = \frac{\gamma K_B}{K\Omega}$$

Where K is the Boltzmann constant.

Table 10 exhibits the [A-G] and the [F-G] parameters. The co-efficients of thermal expansion are also given in this table.

Dynamical Matrix :-

Diagonal $[D_{\alpha'\alpha'}(\vec{q})]$and off diagonal $[D_{\alpha'\beta'}(\vec{q})]$elements of dynamical matrix for the fcc crystal may be written as-

$$D_{\alpha'\alpha'}(\vec{q}) = 4(\beta_1 + 2\alpha_1) - 2(\beta_1 + 2\alpha_1)C\alpha'(C\beta' + C\gamma') - 4\alpha_1 C\beta' C\gamma' + 4\beta_2 S^2\alpha' + 4\alpha_2(S\beta'^2 + S\gamma'_1)$$

$$D_{\alpha'\beta'}(\vec{q}) = 2(\beta_1 - \alpha_1)S\alpha' S\beta'$$

Where α'β' = 1, 2, 3 Cα' = cos(aqα') and Sα' = sin (aqα'), qα' is the α''th component of the phonon wave vector $\vec{q}$ and

$$\alpha_1 = \frac{1}{\gamma_1}\left[\frac{\partial\phi}{\partial\gamma}\right]\gamma_1 . \alpha_2 = \frac{1}{\gamma_2}\left[\frac{\partial\phi}{\partial\gamma}\right]\gamma_2$$

$$\beta_1 = \frac{1}{\gamma_1}\left[\frac{\partial^2\phi}{\partial\gamma_2}\right]\gamma_1 . \beta_2 = \left[\frac{\partial^2\phi}{\partial\gamma^2}\right]\gamma_2$$

Where γ_1 and γ_2 are the separations for the first and the second neighbor respectively.

Table enlists the computed forces constants α_1, α_2, β_1 and β_2 for the solids.

The phonon dispersion :-

The phonon frequency (ν) are obtained by solving the usual secular equation, i.e.,

$$D_{\alpha'\beta'}(\vec{q}) - 4\pi^2\nu^2 mI = 0$$

where m is the mass of atom and I is the unit matrix of 3x3 order. The following dispersion relation along the three major symmetry directions.

Along [100]

$$q_{\alpha'} = q : q_{\beta'} = 0 : q_{\gamma'} = 0$$
$$4\pi^2 m\nu_L^2 = [D_{\alpha'\alpha'}(\vec{q})]_{(100)}$$
$$4\pi^2 m\nu_T^2 = [D_{\beta'\beta'}(\vec{q})]_{(100)}$$

Along [100]

$$q_{\alpha'} = q_{\beta'} = \frac{q}{\sqrt{2}} : q_{\gamma'} = 0$$
$$4\pi^2 m\nu_L^2 = [D_{\alpha'\alpha'}(\vec{q}) + D_{\alpha'\beta'}(\vec{q})]_{(110)}$$
$$4\pi^2 m\nu_{T_1}^2 = [D_{\gamma'\gamma'}(\vec{q})]_{(110)}$$
$$4\pi^2 m\nu_{T_2}^2 = [D_{\alpha'\alpha'}'(\vec{q}) - D_{\alpha'\beta'}(\vec{q})]_{(110)}$$

Along [100]

$$q_{\alpha'} = q_{\beta'} = q_{\gamma'} = \frac{q}{\sqrt{3}}$$
$$4\pi^2 m\nu_L^2 = [D_{\alpha'\alpha'}(\vec{q}) + 2D_{\alpha'\beta'}(\vec{q})]_{(111)}$$
$$4\pi^2 m\nu_T^2 = [D\alpha'\alpha'(\vec{q}) - D_{\alpha'\beta'}(\vec{q})]_{(111)}$$

Table 7, 8 and 9 enlist the percentage contribution of the predicted phonon dispersion for ni, Co and Th respectively. The experimentally measured phonon dispersion due to Bergeneau et al[2]. Furrer and Halg[3], Miller and Brochouse[4], Dutton et al[5]. Sapiro and Moss[6] and Reese et al[7]. Fig. 1, 2, 3, 4, 5 and 6 depict the computed phonon dispersion curves for the solids Ni, Co and Th respectively that gives better result.

Results :-

Phonon dispersion essentially depends on the ensuring interaction; therefore the validity of the main and dominant interaction is well tested by satisfactory agreement between the measured and predicted phonon dispersion in Ni, Co and Th overall agreement of our prediction may be seen better and satisfactory than those given by the simple first principle calculations, which actually deals with the linear response of electrons towards the ionic excitations.It is thus established that the Morse potential in its original form is capable of explicating the said response.**Table – 1**

S. No.	Solids	Bulkmodulas (K) in × 10^{12} dyne-cm^{-2}	Cohesive energy (ϕ) × 10^{-2} ergs	Semi lattice constant in A^0
i	Ni	1.860	7.104	1.760
ii	Co	1.717	7.024	1.775
iii	Th	0.543	9.920	2.540

Table – 2

S. No.	Solids	D (×10^{-12} ergs)	α $\left(A^{0^{-1}}\right)$	γ $(A^0)^0$
i	Ni	0.8006	1.6392	2.6091
ii	Co	0.7790	1.5988	2.6370
iii	Th	0.9267	0.9541	3.8642

Table – 3

S. No.	Solids	C_{11} Model Prediction	Expt 1	C_{12} Model Prediction	Expt 1	Reference No. to the Expt. Values
i	Ni	2.061	2.500	1.537	1.500	Rayne[8]
ii	Co	1.963	2.210	1.470	1.470	Sapiro and Moss[6]
iii	Th	0.718	0.753	0.466	0.489	Aurad[12]

Table – 4

S. No.	Solids	C_{111} Present prediction	C_{111} Prediction of other investigator	C_{112} Present prediction	C_{112} Prediction of other investigator	C_{123} Present prediction	C_{123} Prediction of other investigator	Reference to other studies
i	Ni	-17.073	-21.840	-11.728	-13.450	1.043	0.590	Sharma & Reddy[1]
			-13.575		-8.286		0.721	Mathur et al[14]
			-14.370		-10.530		1.190	Hiki & Granto[15]
			-14.370		-10.530		1.190	Rose[16]
ii	Co	-4.897	-5.470	-3.107	-3.160	+0.171	0.720	Suzuki[17]
			-6.240		-3.820		0.860	Suzuki[17]
			-4.210		-2.420		0.640	Zhdanov etal[1]

			-5.220		-2.480		0.380	Zarochenster et al[19]
			-6.070		-1.280		0.171	Mathur and Gupta[20]
			-4.276		-2.780		0.165	Sharma and Mathur[21]
iii	Th	-04.56		-3.122		+0.292		

Table – 5

The fourth order elastic constants ($\times 10^{12}$ dyne-cm^{-2})

S. No.	Solids	C_{1111}	C_{1112}	C_{1122}	C_{1123}	Reference to other studies
i	Ni	130.510	78.029	88.759	-3.232	Rose[16]
ii	Co	117.4318	74.5994	80.3639	-3.0191	
iii	Th	28.1952	18.0631	20.3355	-1.1124	

Table – 6

The pressure derivatives of the SOEC

S. No.	Solids	∂Ce/∂P		∂K/∂P		∂Cs/∂P		Reference to other studies
		Present Calculation	Other Calculation	Present Calculation	Other Calculation	Present Calculation	Other Calculation	
i	Ni	0.712	0.174	5.539	3.714	3.064	0.390	Mathur el al[66]
ii	Co	0.592		5.239		2.844		
iii	Th	0.391		4.580		2.015		

Table – 7

The A-G, F-G parameters and the co-efficient of thermal expansion

S. No.	Solids	A-G parameters (∂)		F-G parameters	Co-efficoent of thermal expansion		Reference to Expt. Values of
		From elastic const	From pressure derivatives	(γ)	Present study $\times 10^{-6}/^0C$	Expt values	α
i-	Ni	3.737	3.731	3.195	0.079	13.100	George etal[23]
ii-	Co	4.723	4.723	3.158	0.082		
iii-	Th	3.119	3.119	2.872	0.082		

Table – 8

Computed force constants (× 10^4 dyne-cm^{-1})

S. No.	Solids	α_1	α_2	β_1	β_2
i	Ni	0.14079	0.06538	3.78702	-0.26801
ii	Co	-0.13656	0.06256	3.53489	-0.24765
iii	Th	-0.09254	0.03664	1.74193	-0.09864

Table – 9

Percentage contribution of computed phonon dispersion in Ni

	(100)		(110)			(111)	
q	ν_L	ν_T	ν_L	ν_{T1}	ν_{T2}	ν_L	ν_T
0.1	74.00	-	89.74	-	106.17	87.86	88.79
0.2	88.10	93.10	92.50	108.10	95.16	94.31	91.69
0.3	84.09	92.20	92.50	108.10	95.16	94.31	91.69
0.4	87.24	92.93	93.37	108.10	97.90	96.71	90.29
0.5	94.18	94.87	96.98	105.20	100.00	97.63	90.09
0.6	93.54	94.72	97.91	102.60	97.30		
0.7	96.22	93.65	97.69	98.03	101.04		
0.8	98.56	93.84	97.37	95.97	98.47		
0.9	100.23	93.90	93.88	93.76	100.93		
1.0	101.87	94.25	-	-	-		

Table – 10

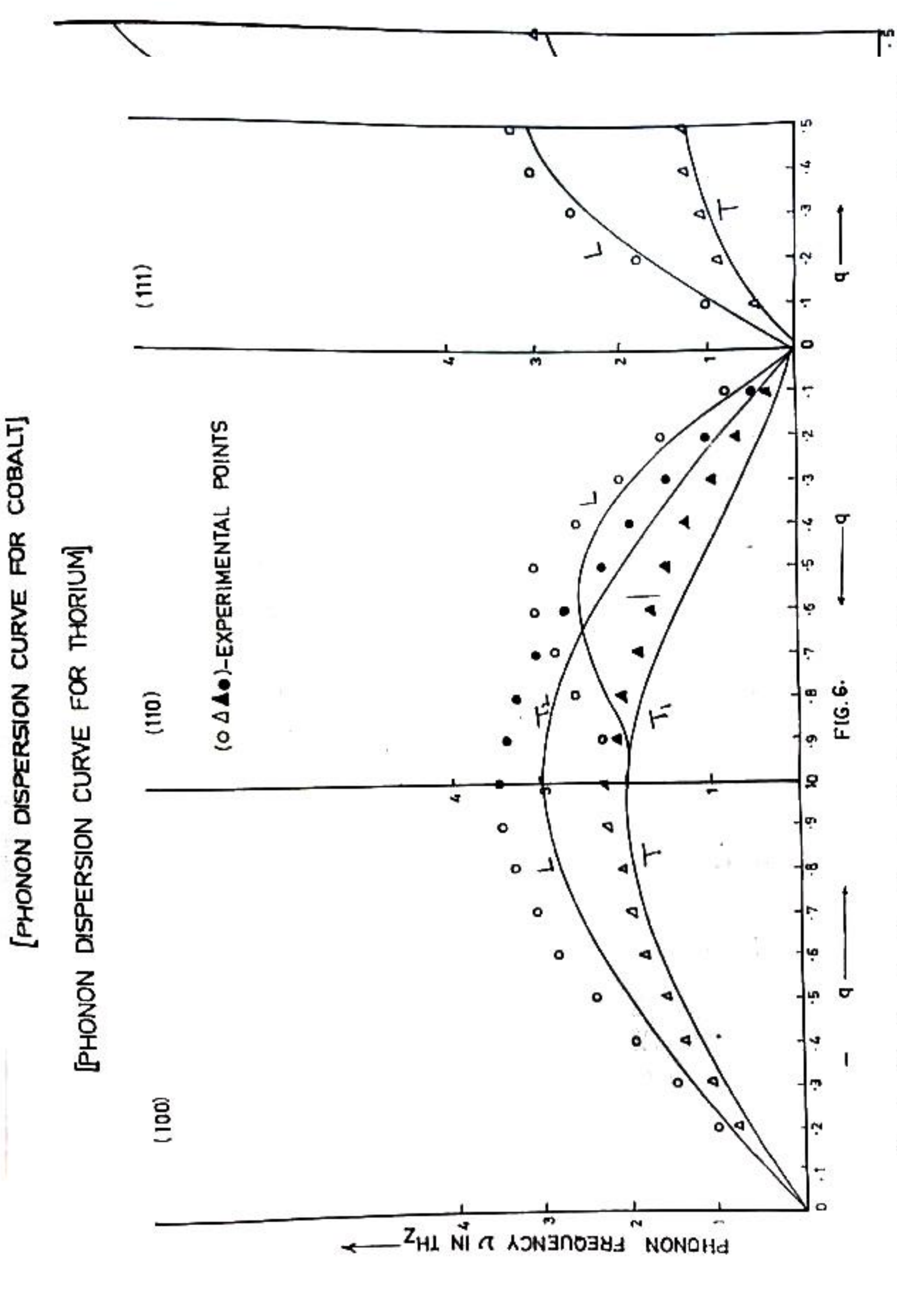
Percentage contribution of computed phonon dispersion in Co

	(100)		(110)			(111)	
q	ν_L	ν_T	ν_L	ν_{T1}	ν_{T2}	ν_L	ν_T
0.1	-	-	98.68	-	86.02	98.69	85.50
0.2	83.44	115.90	91.85	125.15	87.73	88.39	-
0.3	-	-	93.49	116.28	-	88.09	90.90
0.4	88.27	88.26	-	-	90.54	-	91.52
0.5	-	90.82	92.90	-	-	103.36	95.09
0.6	94.47	-	-	-	-		
0.7	-	-	94.70	105.741	96.70		
0.8	-	-	91.60	-	-		
0.9	-	-	-	-	-		
1.0	108.65	96.13	-	-	-		

Table – 11

Percentage contribution of computed phonon dispersion in Th

	(100)		(110)			(111)	
q	ν_L	ν_T	ν_L	ν_{T1}	ν_{T2}	ν_L	ν_T
0.1	-	-	87.03	-	83.48	86.63	84.30
0.2	84.79	84.00	88.44	72.89	84.04	93.34	87.88
0.3	85.81	85.90	93.21	72.74	84.79	94.02	92.61
0.4	85.56	87.24	87.45	74.31	88.41	92.01	98.29
0.5	83.57	89.58	82.13	82.00	90.39	91.35	99.29
0.6	82.91	87.69	81.83	89.51	88.00		
0.7	84.09	89.02	87.14	92.36	84.65		
0.8	83.06	87.58	84.17	90.90	84.03		
0.9	83.96	86.94	86.62	92.90	84.05		
1.0	84.62	86.95	86.76	86.76	84.62		


[PHONON DISPERSION CURVE FOR COBALT]
[PHONON DISPERSION CURVE FOR THORIUM]
(o Δ ▲●)-EXPERIMENTAL POINTS
(100)
(110)
(111)
PHONON FREQUENCY ν IN THz
FIG. 6.
FIG. 5.

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