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RESEARCH ARTICLE

LATTICE DYNAMICAL STUDY OF TITANIUM (Ti) BY USING CGW-VTBFS MODEL

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Abstract

In measurements of the phonon dynamics of bcc Titanium (Ti), In the present paper we have reported the lattice dynamical calculations which are performed by using the Clark-Gazis-Wallis (CGW) and Van der Waalsthree body force shell model (VTBFS).The theory is used to compute the phonon dispersion curves(PDC), the Specific heat variation &frequency distribution with the used temperature. The frequencies along the symmetry directions have plotted against the wavevector to obtain the phonon dispersion curves(PDC)from the present models, with the help of available experimental values. The obtained results are agreed well with experimental data.

Introduction:-

Titanium is a lustrous transition metal which is silver in colour. It possesses low density, high strength, and heat resistance. Titanium alloys are resistant to corrosion, chemicals, and heat. At the low temperature, all metals of groups III-IV transform first and second phase to hcp(α)[1-2] structure at room temperature. Theself-diffusion behaviour ofstable bcc transition metals is also reflected [3,4]. The phonon frequencies of Ti in bcc phase, has been reported by Sexanaet al. [5]. The present work is the second theoretical and the first Angular Force model application on the lattice dynamics of bcc Ti. In this work, an angular force model (CGW), originally proposed by Clark- Gazis-Wallis [6] and later improved by Moore[7]& Upadhyaya et al[8], is used to reproduce the phonon frequencies of bcc Ti. According to this model the angular forces arise due to a change in the angle included between the pair of bonds connecting two neighbours. The changes in the angles of a triangle have been evaluated by making a comparison between the triangle formed by the equilibrium position of these atoms and the projection of the deformed triangle on to the equilibrium planeas shown in Fig. (A)

Theory:

The general formalism of VTBFS model can be derived from the crystal potential whose relevant expression per unit cell is given by

$$\Phi^{C}+\Phi^{R}+\Phi^{TBI}+\Phi^{VWI} \quad (1)$$

First term Φ^{C} is Coulomb interaction potential. This interaction potential is long-range in nature. Thus, total Coulomb energy for the crystal is

$$\Phi^{C}(r)=\sum_{j}{}'\Phi^{C}\alpha_{M}\frac{Z^{2}e^{2}}{r_{0}}\left(r_{ij}\right)$$

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where α_m is the Madelung constant and r_0 is the equilibrium nearest neighbour's distance. Second term Φ^R is short-range overlap repulsion potential.

$\Phi^R(r_{ij}) = ar_{ij}^{\ n}$ (Born Potential) and

$\Phi^R(r_{ij}) = b\exp.(-r_{ij}/\rho)$ (B-M) Potential)

where, a (or b) and η(orρ) are the Born exponents called the strength and hardness parameters, respectively. As a natural consequence of the anti-symmetry requirement on the wave function [12], this alteration in the electronic charge density causes a charge depletion which depends on the inter nuclear separation and interacts with all other charges via Coulomb force law and gives rise to long-range TBI introduced by Lowdin[13] and Lundqvist[14]. This interaction potential is expressed as

$$\Phi^{TBI} = \alpha_m \frac{Z^2e^2}{r_0}\left[\frac{2n}{Z} f(r)_0\right]$$

where, the term $f(r)_0$ is a function dependent on the overlap integrals of the electron wave-functions. Φ^{TBI} is also long-range in nature hence it is added to the $\Phi^{C.}$ and last term Φ^{VWI} is van der Waals interaction potential and owes its origin to the correlations of the electron motions in different atoms closely the method used by Wood et.al[9]. By using the potential energy expression (1), the equations of motion of two cores and two shells can be given as.

$$\omega^2 MU = (R + Z_m C' Z_m)U + (T + Z_m C' Y_m)W \quad (2)$$

$$0 = (T^T + Y_m C' Z_m)U + (S + K + Y_m C' Y_m)W \quad (3)$$

All the variables of eq.(2) & (3) are as described in[10-11].The introduction of VWI and TBI in the framework of RSM with the elimination of W from eqs (2) and (3) leads to the secular determinant:

$$\left|\underline{D}(\vec{q}) - \omega^2 \underline{M}\underline{I}\right| = 0 \quad (4)$$

Let 'o' be the reference atom which has its two neighbors n and n'. Let $\vec{S}_0$, $\vec{S}_n$ and $\vec{S}_{n'}$ be the displacements of the three atoms, respectively. $\hat{e}_{onn'}$ and $\hat{e}_{on'n}$ are taken to be the unit vectors lying in the plane onn' and perpendicular to on and on', respectively. In this model the force on o depends on the change in the angle non'. If the change in this angle is $\Delta\theta$ and corresponding force constant is K, then the potential energy is given by

$\Phi = 1/2K(\Delta\theta)^2 = \frac{1}{2}K\left[\frac{(\vec{S}_0 - \vec{S}_n)\hat{e}_{onn'}}{on} + \frac{(\vec{S}_0 - \vec{S}_{n'})\hat{e}_{on'n}}{on'}\right]^2$ The angular force $\vec{F}_n^{\,A}$ is given by

$$\vec{F}_n^{\,A} = K\left[\frac{(\vec{S}_0 - \vec{S}_n)\hat{e}_{onn'}}{on} + \frac{(\vec{S}_0 - \vec{S}_{n'})\hat{e}_{on'n}}{on'}\right]\left[\frac{\hat{e}_{onn'}}{on} + \frac{\hat{e}_{on'n}}{on'}\right] \quad (5)$$

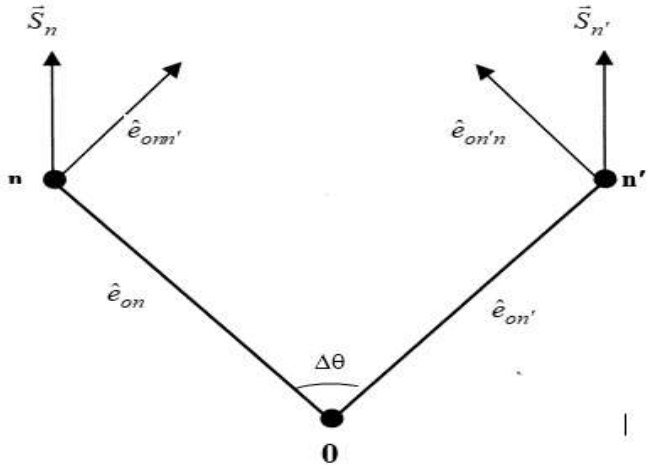

Fig.A:- Clark-Gazis-Wallis(CGW) MODEL.

where the direction of $\hat{e}_{onn'}$ and $\hat{e}_{on'n}$ are such that they reduce the angle non.The restoring force $\vec{F}_n^A$ always lies in the plane non' and its direction is always given by the direction of ($\hat{e}_{onn'}$ /on+ $\hat{e}_{on'n}$ /on).The angular forces of both DAF and CGW types have been employed in case of metals **[15-18]** and results obtained were found to be excellent.These forces have been applied in case of elemental semiconductors **[19-21]** compound semicondu--ctors**[14]**.

Computations:

Specific heats are compared with that computed from the phonon spectra. This comparison is usually done by plotting the specific heat against the temperature. At high temperatures, quantum consideration carries significance changes shown in experimentally but at low temperature the validity of specific heat approximation proved. For calculating the specific heat temperature at low and high temperature case given by formula in eq.(6). In present report the graph at high temperature shows the very small variation but at the lower temperature the sudden large deviation can see which proved more accuracy of the specific heat Vs temperature in comparison with experimental result. The Specific heat constant volume ($C_{V)}$ at temperature T is expressed asDebye's modeldefine the frequency distribution function which is given by

$\Theta_D = h\nu_m / K\,\lambda_{min}$ (6)

For calculating the exact variation ofDebyetemperatures, we have used the Blackmann's [22] sampling technique. In this technique, the frequency spectrum is divided into a suitable number of equal intervals and the specific heat is expressed as a sum over Einstein functions corresponding to the midpoint of each interval. Thus, equation for energy and specific heat are given

$$U = \int_0^{\nu_m} \frac{h\nu^3 VF}{e^{h\nu/kT} - 1}\, d\nu\,, \qquad (7)$$

and

$$C_v = \frac{3R}{6000} \sum_{\nu} g(\nu)E(\nu)d\nu \qquad (8)$$

where E(v) is the Einstein function, R is the gas constant and g(v)dv are the number of frequencies lying in the interval (v-dv/2) to (v+dv/2). In given Figure-3 shows the specific heat variation graph with temperature T.

Table 1:- Input Data [1] and dispersion relation calculated values for bcc Ti.

Input Data		frequency in (Thz) [100]	Frequency max q/q_{max}	frequency in (Thz)[100]	Frequency max q/q_{max}	frequency in (Thz)[110]	Frequency max q/q_{max}
(A˚) M(a.m.u.)	3.315	0.3711	5.0062	2.0627	0.121	0.7876	4.8996
$C_{11}(10^{12}dyn/cm^2)$	47.90	0.5183	6.0813	2.2616	0.8921	0.8382	4.8508
$C_{12}(10^{12}dyn/cm^2)$	1.34	0.5893	4.555	2.3046	1.6117	1.5674	4.7389
$C_{44}(10^{12}dyn/cm^2)$	1.10	0.6334	6.4419	2.4622	2.2116	2.0271	4.4013
$\nu_L(100)(\xi = 1.0)$	0.36	0.7676	5.5293	2.4715	4.3033	2.5451	4.9936
$\nu_L(110)(\xi = 0.5)$	6.30	0.8831	6.1956	2.4857	5.0271	3.2221	3.9236
		1.1741	5.6959	2.6094	4.0122	4.1986	4.3822
		1.1847	5.8492	2.6643	5.9504	4.4645	3.4641
		1.3290	4.6821	2.6803	2.4350		
		1.4236	5.3477	2.7668	4.8838		
		1.5273	4.9436	1.8598	4.3434		
		1.6613	3.8781	1.9102	3.0713		

Table 2:- In put data ofFrequencydistribution and specific heat .

Frequency (THz)	g(V) in arb.units	T(K)	C_V(Cal\mol.K)
0.3711	5.0062	1.0711	0.05126
0.5183	6.0813	1.4728	0.34370
0.5893	4.5550	1.8410	0.81380
0.6334	6.4419	1.9079	0.93150
0.7676	5.5293	2.2594	1.57911
0.8831	6.1956	2.5941	2.46310
1.1741	5.6959	2.8452	3.52510
1.1847	5.8492	3.0962	4.64620
1.3290	4.6821	3.2636	6.00432
1.4236	5.3477	3.4310	7.36240
1.5273	4.9436	3.5481	8.77990
1.6613	3.8781	3.6318	10.1978
1.8598	4.3434	3.7322	11.6746
1.9102	3.0713	3.8494	13.0921
2.0627	0.1210	4.0669	14.3317
2.2616	0.8921	4.3682	15.2751
2.3046	1.6117	4.7531	15.8632
2.4622	2.2116	5.0377	15.9793
2.4710	4.3033	5.1213	14.5603
2.4857	5.0271	5.1883	13.0822
2.6094	4.0122	5.2552	11.6042
2.6640	5.9504	5.4393	10.3617
2.6803	2.4350	5.8243	9.94520
2.7668	4.8838	6.0084	8.64360
2.9041	6.3662	6.1255	7.22420
		6.3264	6.57260
		6.3933	8.04970
		6.4435	9.46780
		6.4770	10.9451
		6.5105	12.4224
		6.5439	13.8996
		6.5774	15.3769
		6.6109	16.8542
		6.6444	18.3315
		6.6778	19.8088
		6.7448	21.2859
		6.8619	21.1077
		6.9121	19.6298
		6.9456	18.1520
		6.9791	16.6742
		6.9958	15.1965
		7.0293	13.7188
		7.0628	12.2410
		7.0962	10.8223
		7.1297	9.34450
		7.1632	7.86670
		7.1967	6.38890
		7.2469	4.91101
		7.2803	3.43324
		7.3473	1.95525
		7.4310	0.53616

Discussions:-

The eight parameter's with elastic constants (C_{11}, C_{12} &C_{44}),six short range force constants a parameters and longitudinal and Transverse mode frequency [1] for (Ti) have reported with phonon dispersion data in Table-1 .The specific heat and density of states data reported in table-2.The Phonon dispersion curve of bcc Titanium is shown in Fig.1the obtained results for the phonon frequencies of bcc Ti in principal symmetry directions are plotted.The calculated frequency distribution and specific heat curves are given in Figure 2, & Figure 3, respectively, and they show the expected behaviours.

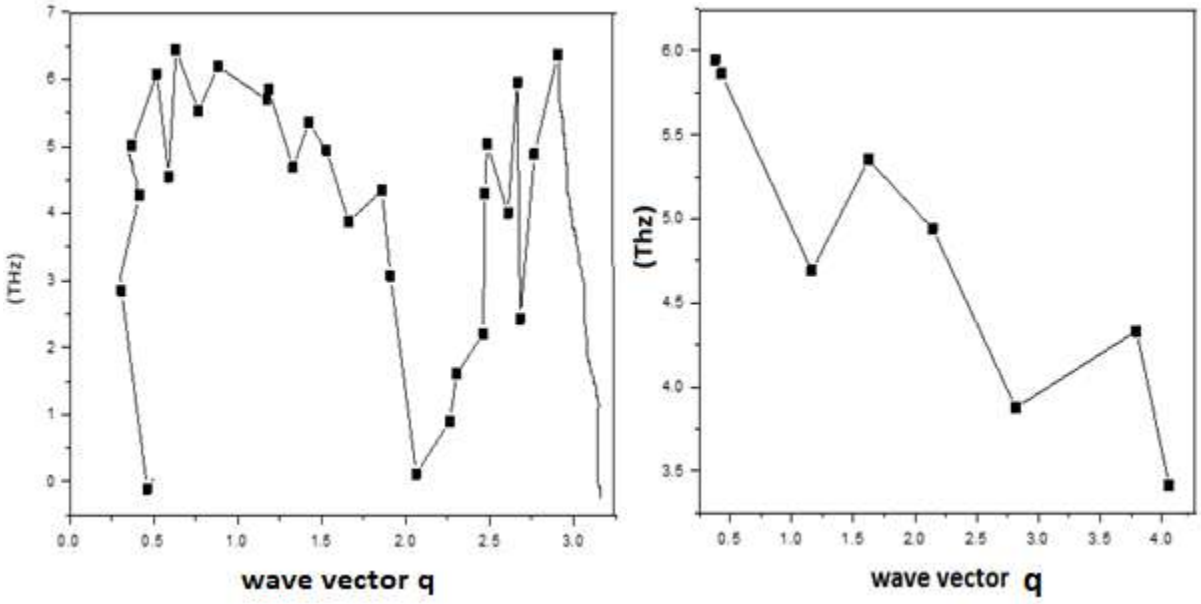

Fig.1:-Phonon dispersion curve of bcc Titanium

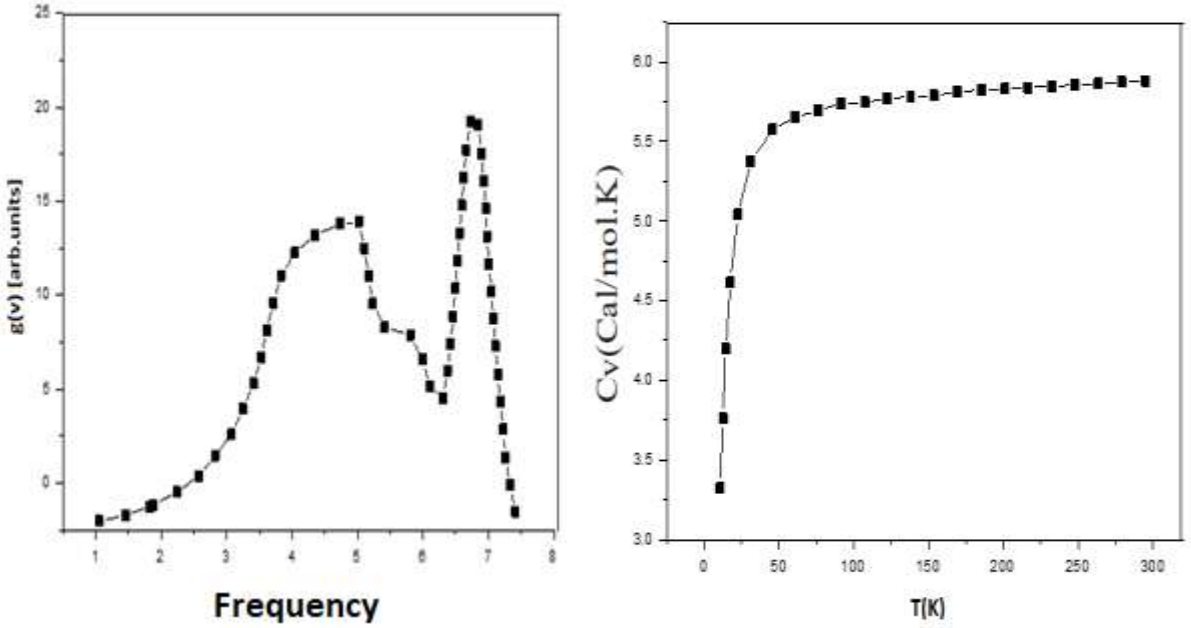

Fig.2:- Frequency distribution curve for bccTitanium.**Fig.3:-** Specific heat curves for bcc Titanium.

Results:-

Useof the present model, the phonon dispersion curves are obtained in Figure 1.The satisfactory description of phonon dispersion relation (PDc) of Tiis exproxmately similar with the theoretical results is given by Sexena et al. [5], exhibit some deviations from experiment, especially, for L(100) and L(110) longitudinal branches. The CGW model in the interaction of three- body force (TB) constant methodis superior to other angular force (AF) methods

because of the three-body interaction. Creep behavior of titanium is investigating in the calculated frequency distribution and specific heat curves, are given in Figure. 2, and Figure. 3 respectively, and it shows the expected behaviours at low and high temperature values.The different researchgroups have been successfully reported theoretical results for other alkali halides, transition metals and semiconducting materials [24-31] by use of the (TBI) and present model. Itis expected that slight discrepancies still occurring between theory and experiment, Van der Waals interactions (if data are available in future) and by including anharmonic vibrations in the present model.

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