DISPERSION OF LATTICE WAVES IN BCC TRANSITION METALS

By B. P. Singh and M. P. Hemkar

Department of Physics, University of Allahabad*

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Recent ideas proposed for the lattice dynamics of fcc transition metals have been further extended to bcc transition metals. The phonon dispersion curves for α-iron and tungsten have been calculated, and it has been shown that almost all the characteristic features are reproduced by the model proposed here. The results obtained are far better than those reported earlier on the basis of different phenomenological models.

1. Introduction

The presence of d-electrons along with the conduction electrons presents a great difficulty in the calculation of lattice vibrational properties of transition metals. A number of attempts have been made to study the lattice dynamics of cubic transition metals on the basis of different phenomenological models [1–4]. The theoretical results based on these models emphasize the need for further studies on the lattice dynamics of transition metals.

A simple but powerful technique has been proposed by Fielek [5] by incorporating the idea of shell for the response of d-electrons to the lattice vibration. In this technique it is assumed that the atoms of the transition metals consist of three entities viz. the outermost conduction electrons, the d-electrons and the remaining ion core. We have applied these ideas quite successfully in the calculation of phonon dispersion relations of noble metals [6] and fcc transition metals [7].

More recently we have improved Fielek's ideas by considering the d-shell-d-shell central interactions up to the second nearest neighbours and applied them in calculating phonon dispersion curves of palladium and platinum [8]. The calculated curves are better than those obtained from Fielek's model. In the present paper we have extended our theory to bcc transition metals and the phonon dispersion curves of α-iron and tungsten have been calculated. The theoretical curves show almost all the fine structure characteristics which are observed in the experimental ones.

* Address: Department of Physics, University of Allahabad, Allahabad-211002, India.

2. Theory

The secular determinant for phonon frequencies $\omega(=2\pi\nu)$ of normal modes of vibration is written in the usual way

$$|D_{ij}(\boldsymbol{q})-4\pi^2\nu^2 MI| = 0, \tag{1}$$

where $i,j = 1, 2, 3$, M is the ionic mass, I is unit matrix of order three and $\boldsymbol{q}$ is a wave vector restricted to the first Brillouin zone (BZ).

The expressions for the natural frequencies in the three major symmetry directions are found to be

[100]−L

$$M\omega^2 = -\tfrac{16}{3}\alpha_1 \sin^2(aq/2)-4\alpha_2 \sin^2(aq)-K+AG(q)+K^2/[K+\tfrac{16}{3}\beta_1 \sin^2(aq/2) +4\beta_2 \sin^2(aq)-A'G(q)], \tag{2a}$$

[100]−T

$$M\omega^2 = -\tfrac{16}{3}\alpha_1 \sin^2(aq/2)-K+AG(q)+K^2/[K+\tfrac{16}{3}\beta_1 \sin^2(aq/2)-A'G(q)], \tag{2b}$$

[110]−L

$$M\omega^2 = -\tfrac{16}{3}\alpha_1 \sin^2(aq/\sqrt{2})-4\alpha_2 \sin^2(aq/\sqrt{2})-K+AG(q)+K^2/[K+\tfrac{16}{3}\beta_1 \sin^2(aq/\sqrt{2}) +4\beta_2 \sin^2(aq/\sqrt{2})-A'G(q)], \tag{2c}$$

[110]−T_1

$$M\omega^2 = -4\alpha_2 \sin^2(aq/\sqrt{2})-K+AG(q)+K^2/[K+4\beta_2 \sin^2(aq/\sqrt{2})-A'G(q)], \tag{2d}$$

[110]−T_2

$$M\omega^2 = -\tfrac{8}{3}\alpha_1 \sin^2(aq/\sqrt{2})-K+AG(q)+K^2/[K+\tfrac{8}{3}\beta_1 \sin^2(aq/\sqrt{2})-A'G(q)], \tag{2e}$$

[111]−L

$$M\omega^2 = -\tfrac{8}{3}\alpha_1 Q_1-4\alpha_2 \sin^2(aq/\sqrt{3})-K+AG(q)+K^2/[K+\tfrac{8}{3}\beta_1 Q_1+4\beta_2 \sin^2(aq/\sqrt{3}) -A'G(q)], \tag{2f}$$

[111]−T

$$M\omega^2 = -\tfrac{8}{3}\alpha_1 Q_2-4\alpha_2 \sin^2(aq/\sqrt{3})-K+AG(q)+K^2/[K+\tfrac{8}{3}\beta_1 Q_2+4\beta_2 \sin^2(aq/\sqrt{3}) -A'G(q)], \tag{2g}$$

where α_1 and α_2 are the radial force constants between nearest and next nearest ion cores, respectively. β_1 and β_2 are the force constants for nearest and next nearest neighbours d-shell-d-shell central interactions. A and A' are the force constants appearing in the ion core-conduction electrons and d-shell-conduction electrons interactions respectively when the Krebs [9] technique is used. K is an isotropic force constant for ion core-d-shell interactions. The expressions for Q_1, Q_2 and $G(\boldsymbol{q})$ are given below

$$Q_1 = 1-\cos^3(aq/\sqrt{3})+2\sin^2(aq/\sqrt{3})\cos(aq/\sqrt{3}), \tag{3a}$$

$$Q_2 = 1-\cos^3(aq/\sqrt{3})-\sin^2(aq/\sqrt{3})\cos(aq/\sqrt{3}), \tag{3b}$$

and

$$G(q)_{ij} = \sum_{h} \left[\frac{(q_i+h_i)(q_j+h_j)}{|q+h|^2+(a/\pi)^2 k_c^2} \, g^2(B|q+h|) - \frac{h_i h_j}{h^2+(a/\pi)^2 k_c^2} \, g^2(B|h|) \right], \tag{4}$$

where a is semi lattice parameter, h is the reciprocal lattice vector, k_c is Bohm–Pine [10] screening parameter, B is the Wigner–Seitz radius and $g(x)$ is given by

$$g(x) = 3(\sin x - x\cos x)x^{-3}, \text{ and } x = B|q+h|. \tag{5}$$

If we neglect ion core-conduction electrons interaction, the remaining force constants involved in equations (2) for lattice frequencies are determined from experimental elastic constants and three zone boundary frequencies. The equations used in the evaluation of force constants are

$$\alpha_1+\beta_1 = -3aC_{44}, \tag{6a}$$

$$\alpha_2+\beta_2 = -a(C_{11}-C_{12}), \tag{6b}$$

$$A' = 4a^3(C_{12}-C_{44})k_c^2, \tag{6c}$$

$$4\pi^2 M\nu_L^2(100)+\tfrac{16}{3}\alpha_1+K = K^2/[K+\tfrac{16}{3}\beta_1-A'G_{11}(100)], \tag{6d}$$

$$4\pi^2 M\nu_{T_2}^2(\tfrac{1}{2}\,\tfrac{1}{2}\,0)+\tfrac{8}{3}\alpha_1+K = K^2/[K+\tfrac{8}{3}\beta_1-A'G_{33}(\tfrac{1}{2}\,\tfrac{1}{2}\,0)], \tag{6e}$$

$$4\pi^2 M\nu_L^2(\tfrac{1}{2}\,\tfrac{1}{2}\,0)+\tfrac{16}{3}\alpha_1+4\alpha_2+K = K^2/[K+\tfrac{16}{3}\beta_1+4\beta_2-A'\{G_{11}(\tfrac{1}{2}\,\tfrac{1}{2}\,0)+G_{12}(\tfrac{1}{2}\,\tfrac{1}{2}\,0)\}]. \tag{6f}$$

The experimental input parameters for α-iron and tungsten are listed in Table I and the calculated values of force constants in Table II.

TABLE I

Experimental input parameters (elastic constants in units of 10^{10} Pa and lattice constant in Å)

Metal	Elastic constants			Lattice constant (2a)	Reference	Zone boundary frequencies (THz)		
	c_{11}	c_{12}	c_{44}			$\nu_L(100)$	$\nu_{T_2}(\frac{1}{2}\frac{1}{2}0)$	$\nu_L(\frac{1}{2}\frac{1}{2}0)$
α-iron	23.31	13.55	11.78	2.8662	[17]	8.56	6.40	9.19
Tungsten	52.327	20.453	16.072	3.165	[18]	5.6	4.40	6.75

TABLE II

Calculated values of force constants (10^3 dyn cm^{-1})

Metal	α_1	α_2	β_1	β_2	K	A'
α-iron	−50.4962	−14.31	−0.1496	0.3229	0.5992	18.4702
Tungsten	−74.2126	−51.9419	−2.0892	1.5013	7.4831	70.2345

3. Results and discussion

1. α-iron: The phonon dispersion for this ferromagnetic metal has been experimentally studied through inelastic neutron scattering by many workers. Recently Minkiewicz et al. [11] have presented a detailed study of phonon dispersion at 295 K for phonon wave vectors along the three highly symmetry directions. Their measurements agree well with those of Brockhouse et al. [12]. In Fig. 1, we have plotted our theoretical curves along with the experimental values of Minkiewicz et al. as these extend over the entire Brillouin zone (BZ). There is an excellent agreement between the theoretical and experimental curves.

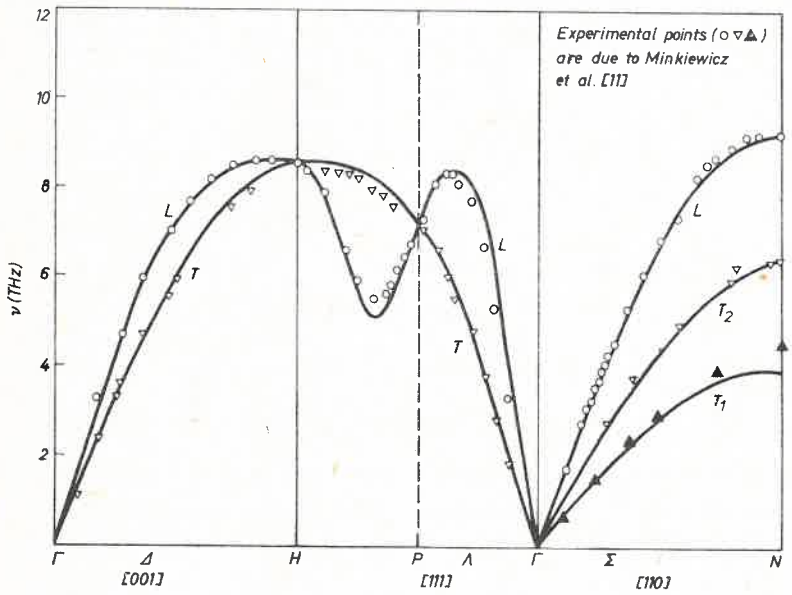

Fig. 1. Phonon dispersion curves of α-iron at 295K along indicated directions. Full curves represent the theoretical findings

2. Tungsten: Chen and Brockhouse [13] have measured the frequency versus wave vector dispersion relations at room temperature for lattice waves travelling in the three highest symmetric directions from the momentum and energy changes in the inelastic scattering of slow neutrons. Their experimental points are plotted in Fig. 2 along with their calculated values. In the present calculations, the next nearest neighbours radial force constant between ion cores is fairly large as predicted by Chen and Brockhouse. It can be seen from the figure that our calculated results are in broad agreement with experimental data except for some deviations in Δ_L and Λ_L branches for large values of wave vectors.

Our results are also better than those of Shukla and Cavalheiro [14], Gupta and Hemkar [15] and Shukla and Padial [16] derived from different phenomenological models. However, as things stand, the proposed model gives an adequate description of lattice

waves dispersion in bcc transition metals. The existing discrepancies may, however, be attributed to a) the neglect of ion core-ion core angular interactions, b) the neglect of flexibility of d-orbitals, c) the neglect of ion core-conduction electrons interactions, d) the choice of dielectric function (in the present calculations Lindhard dielectric function is used).

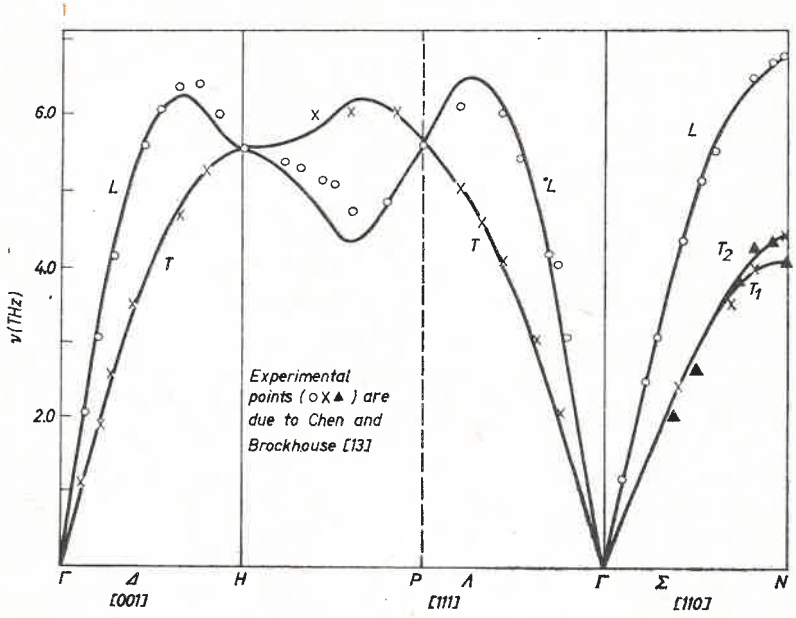

Fig. 2. Phonon dispersion curves of tungsten at room temperature along indicated directions. Full curves represent the theoretical findings

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