DYNAMICAL THEORY OF THE VIBRATION SPECTRA OF CRYSTALS

Part IV. The Metallic Crystals

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1. Introduction

Most metals crystallise in the cubic system with either the face-centred or the body-centred structure and consequently it is of importance to investigate the vibration spectra of these structures. The methods of the foregoing papers have therefore been applied here to derive expressions for the frequencies of the eigenvibrations of the above two structures.

2. The Face-centred Cubic Lattice

The vibration spectrum of this structure has already been described as consisting of four independent modes, *viz.*, the normal and tangential oscillations of the octahedral planes of atoms and the normal and tengential oscillations of the cubic planes of atoms with degeneracies of 4, 8, 3 and 6 respectively. The influence of the 12 nearest neighbours (atoms 1 to 12) surrounding every atom in the structure can be represented by three independent force constants Q, R and S and that of the next nearest neighbours (atoms 13 to 18) by two independent constants T and U. The six constants including P, the force on any atom proportional to its own displacement, are described in Table I.

The condition that an infinitesimal translation of the entire structure involves no work done, results in the relation

$$P + 4Q + 8R + 2T + 4U = 0$$

between the force constants. The expressions for the frequencies of the four eigenvibrations are contained in Table II.

From Table I it can be seen that Q and U will be negligible in comparison with the other constants. R and S will be of the same order of magnitude, but $R > S$ in a valence structure, since the former is a longitudinal and the latter a transverse force. It is also evident that $P > (-8R)$. So

TABLE I

Description of the Force Constants

Atoms responsible for forces	Symbol	Description
0	P	Force on any atom proportional to its own displacement
1 to 12	Q	Force and displacement perpendicular to the cabic plane containing the two atoms
1 to 12	R	Force and displacement along the same cubic axis, the plane containing the two being the cubic plane containing the two atoms
1 to 12	S	Force and displacement along different cube axes, the plane containing the two being the cubic plane containing the two atoms
13 to 18	T	Force and displacement parallel to each other and to the line joining the two atoms
13 to 18	U	Force and displacement perpendicular to the cubic plane containing the two atoms

TABLE II

Expressions for the Frequencies of Vibration

Probable Sequence	Degeneracy	Oscillating Units	Direction of oscillation	$4\pi^2\nu^2c^2\ m$
I	3	(100) planes	Normal	P+4Q−8R+2T+4U
II	4	(111) planes	Normal	P−8S−2T−4U
III	6	(100) planes	Tangential	P−4Q+2T+4U
IV	8	(111) plones	Tangential	P+4S−2T−4U

if we neglect the constant T, the order of magnitude of the frequencies will be the same as that shown in Table II. But T being a negative quantity, it is possible that a consideration of this force might bring about a reversal of the order with regard to modes I and II. In any case the vibration spectrum of the face-centred lattice consists of a close doublet with high frequency, one mode with medium frequency and one mode with low frequency.

3. THE BODY-CENTRED CUBIC LATTICE

The vibration spectrum of the body-centred cubic lattice consists of a triply degenerate vibration of the two interpenetrating cubic lattices against each other and three vibrations of alternate dodecahedral planes with opposite phases, in three directions, *viz.*, normally, transversely parallel to

a cube axis, and transversely along the dodecahedral axis in the plane, with degeneracies of 6 each. The interaction of every atom in the structure with its eight nearest neighbours (atoms 1 to 8) can be represented by two constants Q and R and that with the next nearest neighbours by the constants S and T. So we have four independent constants in addition to the force P on any atom proportional to its own displacement. The constants are described in Table III.

TABLE III

Description of Force Constants

Atoms responsible for forces	Symbol	Description
0	P	Force on any atom proportional to its own displacement
1 to 8	Q	Force and displacement parallel to each other and along a cube axis
1 to 8	R	Force and displacement perpendicular to each other and along different cube axes
9 to 14	S	Force and displacement perpendicular to the cubic plane containing the two atoms
9 to 14	T	Force and displacement parallel to each other and to the line joining the two atoms

The condition that a translation of the crystal has zero frequency leads to

$$P + 8Q + 4S + 2T = 0$$

The frequencies of the modes obtained in terms of the constants are contained in Table IV.

TABLE IV

Expressions for the Frequencies of Vibration

Probable Sequence	Degeneracy	Oscillating Units	Direction of oscillation	$4\pi^2\nu^2c^2m$
I	3	Body centre atoms against cube corner atoms	Arbitrary	P−8Q+2T+4S
	6			
II		(011) planes	[011]	P−8R−2T
III	6	(011) planes	[100]	P+2T−4S
IV	6	(011) planes	[01$\bar{1}$]	P+8R−2T

In this case the quantity S will be negligible, as can be inferred from its description in Table III. If we further neglect T, then P = − (8Q) and also

$Q > R$ for the reason that the former is a longitudinal force and the latter a transverse force, the directions of the line joining the interacting atoms being along the trigonal axes. The order of magnitudes of the frequencies will therefore be the same as that shown in Table IV. But, here again, the consideration of T which is negative, may possibly reverse the order so far as modes I and II are concerned. The spectrum consists of two high frequencies, one medium and one very low frequency.

In conclusion the author's grateful thanks are due to Prof. Sir C. V. Raman for his kind interest in the work.

SUMMARY

Exact expressions have been derived for the frequencies of the eigenvibrations of the face-centred and body-centred cubic lattices in terms of 6 and 5 force constants respectively, the constants in each case being connected by one additional relation.