MODES OF VIBRATION OF THE HEXAGONAL CLOSE-PACKED LATTICE

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1. *Introduction*

The hexagonal close-packed structure is a frequently encountered atomic arrangement in the crystalline form of many metallic elements. It is associated with a hexagonal unit cell having the axial ratio c/a equal to 1·63, and is a closest packing of spheres. The unit cell contains two atoms which have the co-ordinates 0, 0, 0; 2/3, 1/3, 1/2. In some metals, the axial ratio is slightly different from 1·63, but the co-ordinates of the atoms is the same. In this paper, the modes of vibration of the hexagonal close-packed structure are investigated on the basis of the fundamental ideas proposed by Sir C. V. Raman in an earlier paper. The results are true for any hexagonal structure in which there are atoms at 0, 0, 0; 2/3, 1/3, 1/2 and is not restricted to the case where the axial ratio is 1·63.

In a preceding paper, the author has discussed the modes of vibration of a simple hexagonal Bravais lattice, and has shown that the eight types of vibration fall into four sets, namely (+ + +); (+ + −); (+ − +, − + +, − − +); (+ − −, − + −, − − −). We shall now take up each of these sets, and discuss the modes of the close-packed lattice under it, using group theoretical methods. In this connection, it must be noted that the crystal belongs to the space-group D^4_{6h}, in which the inversion is not at a lattice point, but is at a point midway between the two atoms, *i.e.*, at 1/3, 1/6, 1/4. Hence, the method used by E. V. Chelam in an earlier paper in discussing the vibration of the diamond lattice is employed for deriving the character table and the modes of vibration.

2. *The* (+ + +) *and* (+ + −) *Types of Vibration*

We first consider the two atoms in the unit cell to be different, so that there is no centre of inversion. Then, the group of the vibration (*cf.* earlier paper by the author) is D_{3h}, whose character table is drawn up below. The reduced character ψ (R) for each of the operations in the + + + type is tabulated below against ψ_{+++}. Thus, two vibrations (coupled) are

obtained under A_2'' and two others coupled under E'. On introducing the centre of inversion, the coupling is removed, the modes splitting up into two, symmetric and antisymmetric with respect to inversion. Also, it is easily seen that these modes are distinct. They represent the three translations of the lattice as a whole, and three vibrations of the two interpenetrating lattices against one another, one being along the hexagonal axis and the other two degenerate in the perpendicular plane.

D_{3h}	E	σ_h	$2C_3$	$2S_3$	$3C_2$	$3\sigma_v$	n_i (+ + +)	n_i (+ + −)
A_1'	1	1	1	1	1	1	..	1
A_2'	1	1	1	1	−1	−1	..	..
A_1''	1	−1	1	−1	1	−1	..	..
A_2''	1	−1	1	−1	−1	1	2	1
E'	2	2	−1	−1	0	0	2	1
E''	2	−2	−1	1	0	0	..	1
ψ_{+++}	6	2	0	−4	−2	2		
ψ_{++-}	6	0	0	0	0	2		

Coming to the + + − type of vibration, it has been shown by the author (*loc. cit.*) that for the simple hexagonal lattice, the group of the vibration is D_{6h}. In the present case, if we consider the two atoms to be distinct, there is no centre of inversion, and the group is only D_{3h}, which is the same as for + + +. The reduced character for this is tabulated in the character table against ψ_{++-} and the number of modes n_i under each state is determined. It is found that there is one mode each under A_1', A_2'', E' and E''. On introducing the centre of symmetry, and associating it with the operations of the group D_{3h}, the translation operators are brought in thus:

$$i\sigma_h i^{-1} = \sigma_h\tau_z;\ iC_3i^{-1} = C_3\tau_x;\ iS_3i^{-1} = S_3\tau_x\tau_z;\ iC_2i^{-1} = C_2\tau_x\tau_z;\ i\sigma_v i^{-1} = \sigma_v\tau_x.$$

Hence, the operations of D_{3h} do not commute with the inversion, and the group $D_{3h} \times i$ contains the product of the operations of D_{3h} and the translations. It has been shown by Chelam (*loc. cit.*) that the character of the product of an operation R of the point-group and a translation T is the product of their characters, *i.e.*, $\chi(RT) = \chi(R)\ \chi(T)$. Thus, on introducing the inversion, the following transformations occur:

$\chi(\sigma_h) \rightarrow -\chi(\sigma_h)$; $\chi(C_3) \rightarrow \chi(C_3)$; $\chi(S_3) \rightarrow -\chi(S_3)$; $\chi(C_2) \rightarrow -\chi(C_2)$ and $\chi(\sigma_v) \rightarrow \chi(\sigma_v)$. Hence, the representations A_1' and A_2'' are sent one into the other and so are E' and E''. Thus these are equivalent under the inversion and give rise respectively to a double and a quadruple representation in the space-group. Thus, the vibrations symmetric and antisymmetric

with respect to the inversion are identical. Hence, under this type, we have a vibration along the hexagonal axis with degeneracy 2, and another degenerate in the perpendicular plane with degeneracy 4.

3. *The Remaining Types of Vibration*

The vibration represented by the set $(+\ -\ +,\ -\ +\ +,\ -\ -\ +)$ denotes the vibration of atoms in alternate prismatic planes. Taking one of them, $+\ -\ +$, it is easily seen that the group of the vibration is only C_{2v}, if the two atoms are considered distinct. The character table is given below. The transformations on introducing the inversion are $iC_2i^{-1} = C_2\tau_x\tau_z$; $i\sigma_v i^{-1} = \sigma_v\tau_x$; $i\sigma_v' i^{-1} = \sigma_v'\tau_z$. These keep the representations invariant, so that each of them splits into two, one symmetric and the other antisymmetric, with respect to the inversion. In these, the successive atomic planes have the phases $+\ -\ -\ +$ and $+\ +\ -\ -$ respectively. These are distinct since the planes are not equally spaced.

C_{2v}	E	C_2	σ_v	σ_v'	n_i $(+\ -\ +)$	n_i $(+\ -\ -)$
A_1	1	1	1	1	2	2
B_2	1	−1	−1	1	2	1
A_2	1	1	−1	−1	..	1
B_1	1	−1	1	−1	2	2
$\psi\ +\ -\ +$	6	−2	2	2		
$\psi\ +\ -\ -$	6	0	2	0		

The last set $(+\ -\ -,\ -\ +\ -,\ -\ -\ -)$ represents vibrations of atoms in diagonal planes of the type $(01\bar{1}1)$. For this also, the group of the vibration is C_{2v} and taking one of the types, $+\ -\ -$, the values of ψ and n_i are shown in the above character table. Using the transformations in the previous paragraph, it is seen that the representations A_2 and B_2 become equivalent, and so do A_1 and B_1. Thus, we get a doubly degenerate vibration antisymmetric to σ_v, and two coupled doubly degenerate vibrations symmetric to it. The direction of the former is parallel to the plane and perpendicular to the hexagonal axis. It may also be described as the intersection of the vibrating plane with the horizontal reflection plane of the lattice. The other two vibrations take place in, two unspecifiable directions in the perpendicular plane σ_v. A physical explanation for the equivalence of the symmetrical and antisymmetrical modes consists in the fact that the vibrating planes may be imagined to be either the $(01\bar{1}1)$ or the $(01\bar{1}\bar{1})$ planes.

The modes of vibration may thus be described as follows:—

No.	α β γ	*Description*	*Number of modes*
1, 2	+ + +	Translation of the lattice as a whole	1, 2
3	+ + +	Vibration of the atoms in the two lattices against each other, in a direction parallel to the hexagonal axis Oz	1
4	+ + +	Same as (3), but in a plane perpendicular to Oz, the vibration being degenerate in the plane	2
5	+ + −	Vibration of basal (0001) planes with the phases (+ + − −) and (+ − − +) normally	2
6	+ + −	Same as (5), but transversely degenerate in the plane ..	4
7 to 9	+ − +	Vibrations of prismatic planes in three directions,	
	− + +	normally, transversely perpendicular to the hexagonal	
	− − +	axis, and parallel to it, with the phases + + − −	3, 3, 3
10 to 12	do	Same as (7) to (9) but with the phases + − − + ..	3, 3, 3
13	+ − −	Vibration of the $(01\bar{1}1)$, $(10\bar{1}1)$, $(1\bar{1}01)$ planes with	
	− + −	the phases (+ + − −) and (+ − − +) in a	
	− − −	direction in the plane perpendicular to the hexagonal axis	6
14, 15	do	Same as (13), but in two unspecifiable directions in a plane perpendicular to the direction in (13), as described above	6, 6
		Total ..	48
		Number of distinct modes ..	13

In conclusion, I wish to express my grateful thanks to Prof. Sir C. V. Raman for the keen interest that he took in the investigation.

Summary

The modes of vibration of the hexagonal close-packed structure is worked out on the basis of the Raman theory of crystal vibrations. The character tables are drawn up, and the vibrations are derived by a method due to E. V. Chelam without using the character table of the space-group. It is found that there are 13 vibrations with degeneracies 1, 2, 2, 4, 3, 3, 3, 3, 3, 6, 6, 6. The planes which take part in each mode and the directions of vibration for these are also described.

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