It may therefore be concluded that there are good reasons, theoretical as well as practical, why the Fourier method should be used in accurate crystal-structure determinations.

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Vibration Amplitudes of Atoms in Cubic Crystals

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Root-mean square amplitudes of atomic vibration are given for twenty elements and twenty-four compounds crystallizing in the cubic system. The spatial distribution of atomic displacements due to thermal vibration is calculated from the elastic constants of nineteen cubic crystals, and attention is drawn to the relationships existing between the amplitudes of pure longitudinal and transverse waves travelling along the cube edges, face diagonals and cube diagonals, and the structures of these crystals.

From the data given, the intensity of diffuse scattering power could be plotted in reciprocal space, for comparison with experimental data from monochromatic Laue photographs.

It is possible to calculate a root-mean square amplitude of thermal vibration of atoms in cubic crystals if the Debye characteristic temperature is known. But the atoms are not just simple-harmonic oscillators, although their movements are resolvable into a series of harmonic vibrations. The object of the present paper is in § 1 to give the root-mean square amplitudes and in § 2 to investigate the spatial distribution of amplitudes in these component vibrations, and to consider what relation, if any, exists between the amplitudes of waves travelling in certain principal directions and the crystal structure.

1. Root-mean square amplitude of vibration

The Debye-Waller formula, $I_T = Ie^{-2M}$, which was confirmed by early experimenters, applies to cubic crystals composed of one kind of atom only, at temperatures not too near to the melting-point. It expresses the reduction of Bragg scattering of X-rays by crystals with increasing temperature, in terms of the mean square displacement of an atom from the average position which it occupies in the crystal. In this expression M is given by

$$M = \frac{8\pi^2 \sin^2\theta}{3\lambda^2}\,\overline{u^2}. \tag{1}$$

M may, however, also be expressed in terms of Θ, the Debye characteristic temperature of specific heat theory

$$M = \frac{6h^2}{mk\Theta}\,\frac{\sin^2\theta}{\lambda^2}\left\{\frac{\phi(x)}{x}+\frac{1}{4}\right\}, \tag{2}$$

where h, k are the Planck and Boltzmann constants, m the mass of the atom in grams, θ the Bragg angle, λ the wave-length of X-rays, $x = \Theta/T$, where T is the absolute temperature, and $\phi(x)$ is the Debye function of

$$\frac{1}{x}\int_0^x \frac{\xi\,d\xi}{e^{\xi}-1}$$

(which is tabulated, for instance, in the *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935), **2**, p. 574). The term $\frac{1}{4}$ allows for the existence of zero-point energy.

Equating (1) and (2), we find that

$$\overline{u^2} = \frac{9h^2}{4\pi^2 km\Theta}\left\{\frac{\phi(x)}{x}+\frac{1}{4}\right\} = \frac{4{\cdot}364\times 10^{-14}}{A\Theta}\left\{\frac{\phi(x)}{x}+\frac{1}{4}\right\}, \tag{3}$$

where A is the atomic weight in terms of ${}^{16}_{8}\mathrm{O}$, the values of universal constants used being those given by Birge (1941).

Table 1 gives the root-mean square amplitudes at 293° K. calculated from equation (3) for a number of elements crystallizing in the cubic system, using the values of Θ given by Seitz (1940).

Using the same values of Θ, one finds that the root-mean square amplitudes of thermal vibration are reduced to something over one-half the above values at liquid-air temperatures. Actually the characteristic temperature usually increases slightly with lowering of temperature (Blackman, 1935*a*, *b*; Owen & Williams, 1947), but the effect of this is small compared with other uncertainties involved in the calculations. A direct experimental check on the above values by X-ray measurements has been made only in the case of Al, Au and Cu. James, Brindley & Wood (1929) found for Al at 290° K., $\sqrt{(\overline{u^2})}=0{\cdot}171$ A. and at 86° K., $\sqrt{(\overline{u^2})}=0{\cdot}111$ A., which would correspond to $\Theta_{290^\circ}=409{\cdot}5^\circ$ K. and $\Theta_{86^\circ}=415{\cdot}5^\circ$ K. from formula (3). Owen & Williams (1947), by intensity measurements at from 300 to 900° K., obtained room-temperature (293° K.) values of Θ as follows:

$$\Theta_{\mathrm{Al}}=395^\circ\,\mathrm{K.},\quad \Theta_{\mathrm{Au}}=175^\circ\,\mathrm{K.},\quad \Theta_{\mathrm{Cu}}=314^\circ\,\mathrm{K.},$$

agreeing well with the values given by Seitz, which were derived from specific heat data.

In the case of crystals composed of more than one kind of atom, a different value of M applies to each atom; but experiment has shown that the differences in vibration amplitude are not large, in general, even when the atomic weights of the different kinds of atoms are very different. Waller & James (1927) gave values of $\sqrt{(\overline{u^2})}$ for Na^+ and Cl^- in rock-salt, based on measurements of the intensity of reflexion at different temperatures from planes in which the Na and Cl atoms scatter in the same or opposite phases respectively. Wasastjerna (1945) used a different experimental method for a number of alkali halides. He measured the atom-scattering factors of Na^+, F^-, Cl^-, Br^-, I^-, K^+, etc., in the various salts and compared the curves he obtained with the theoretical values given by James & Brindley (1931), thus deducing M for each atom from the relation $f_T=f_0e^{-M}$, and hence $\sqrt{(\overline{u^2})}$. In this way he found a small difference in M even for K^+ and Cl^- in KCl, a difference which had been supposed by James & Brindley (1928) not to exist; James & Brindley obtained $\sqrt{(\overline{u^2})}$ for KCl at two different temperatures, but treated the crystal as if it were a simple cubic structure containing one kind of atom only. The collected experimental results are given in Table 2.

Table 1. *Root-mean square amplitudes of atomic vibration at* 293° K. *for elements crystallizing in the cubic system*

Element	A	Θ	$\overline{u^2}$	$\sqrt{(\overline{u^2})}$	Structure type
Pb	207·2	88° K.	0·080 A.^{2}	0·28 A.	A 1 (f.c.c.)
Ca	40·1	230	0·061	0·25	,,
Sr	87·6	170	0·051	0·23	,,
Al	27·0	390	0·033	0·18	,,
Ag	107·9	215	0·026	0·16	,,
Au	197·2	170	0·023	0·15	,,
Cu	63·6	315	0·021	0·145	,,
Pd	106·7	275	0·016	0·13	,,
Pt	195·2	225	0·013	0·115	,,
Ir	193·1	285	0·008	0·09	,,
K	39·1	100	0·328	0·57	A 2 (b.c.c.)
Na	23·0	150	0·249	0·50	,,
α-Fe	55·9	420	0·014	0·12	,,
Ta	180·9	245	0·012	0·11	,,
Cr	52·0	485	0·011	0·105	,,
Mo	96·0	380	0·010	0·10	,,
W	183·9	310	0·0075	$0{\cdot}08_5$	,,
C (diamond)	12·0	2340	0·0004	0·02	A 4 (diamond)
Ge	72·6	290	0·021	0·145	,,
Sn	118·7	260	0·016	0·13	,,

Table 2. *Root-mean square amplitudes of atomic vibration experimentally determined for alkali halides*

	Wasastjerna				Waller & James				James & Brindley	
Compound	Temp. ° K.	$\sqrt{(\overline{u_a^2})}$ A.	$\sqrt{(\overline{u_b^2})}$ A.	δ A.	Temp. ° K.	$\sqrt{(\overline{u_a^2})}$ A.	$\sqrt{(\overline{u_b^2})}$ A.	δ A.	Temp. ° K.	$\sqrt{(\overline{u^2})}$ A.
NaF	293	Na^+ 0·17	F^- 0·195	0·183	—	—	—	—	—	—
NaCl	293	Na^+ 0·245	Cl^- 0·235	0·239	86	Na^+ 0·152	Cl^- 0·133	0·141	—	—
					290	Na^+ 0·242	Cl^- 0·217	0·227	—	—
					500	Na^+ 0·315	Cl^- 0·283	0·296	—	—
KCl	293	K^+ 0·27	Cl^- 0·26	0·265	—	—	—	—	86	0·149
									290	0·255
KBr	293	K^+ 0·28	Br^- 0·27	0·273	—	—	—	—	—	—
KI	293	K^+ 0·32	I^- 0·30	0·305	—	—	—	—	—	—
RbCl	293	Rb^+ 0·26	Cl^- 0·26	0·26	—	—	—	—	—	—
CsI	293	—	—	0·33	—	—	—	—	—	—

In this table the 'observed amplitude' δ is computed from $\sqrt{\{(m_a\overline{u_a^2}+m_b\overline{u_b^2})/(m_a+m_b)\}}$, and it will be seen that the maximum differences between δ and $\sqrt{(\overline{u_a^2})}$ or $\sqrt{(\overline{u_b^2})}$ are of the order of 7%. This being so, it seems justifiable to use equation (3) for the calculation of values of $\sqrt{(\overline{u^2})}$ for cubic compounds for which Θ is known, on the assumption that they are composed of only one kind of atom, of atomic weight

$$A=(m_a+m_b+\ldots+m_n)/n.$$

The errors introduced in this way are probably less than those involved in uncertainty in the values of Θ. Seitz gives a few values of Θ for compounds, and some further values can be deduced from available specific heat data, as given in the *Landolt-Börnstein* or the *International Critical Tables*. (A good outline of methods is given by Roberts (1940).) Wasastjerna (1935, 1938) has calculated the values of $\sqrt{(\overline{u^2})}$ for a number of alkali halides from the potential of repulsion in the crystalline state, but his subsequent experimental investigation (1945) of certain of these compounds indicated that the calculated root-mean square amplitudes were all about 13% too low. His corrected figures are included in Table 3, together with the corresponding deduced characteristic temperatures (inserted in brackets). All data refer to a temperature of 293° K.

Table 3. *Root-mean square amplitudes of atomic vibration at 293° K. calculated and observed for various cubic crystals*

Compound	A	Θ °K.	$\overline{u^2}$ A.	$\sqrt{(\overline{u^2})}$ A.	Remarks and references
NaF	21·00	439	0·034	$0{\cdot}18_5$	Θ from Debye's specific heat function
NaCl	29·23	281	0·057	0·24	Seitz, from specific heats
NaBr	51·46	(200)	0·063	0·25	Wasastjerna, from potential of repulsion
NaI	74·97	(151)	0·075	$0{\cdot}27_5$	Do.
KF	29·05	(321)	0·045	0·21	Do.
KCl	37·28	227	0·068	0·26	Seitz, from specific heats
KBr	59·51	177	$0{\cdot}069_5$	$0{\cdot}26_5$	Do.
KI	83·01	(132)	0·093	$0{\cdot}30_5$	Wasastjerna, observed $\overline{u^2}$ by X-rays
RbF	52·22	(238)	$0{\cdot}045_5$	0·21	Wasastjerna, from potential of repulsion
RbCl	60·45	(179)	$0{\cdot}067_5$	0·26	Wasastjerna, observed $\overline{u^2}$ by X-rays
RbBr	82·68	(140)	0·084	0·29	Wasastjerna, from potential of repulsion
RbI	106·2	(110)	$0{\cdot}100_5$	0·32	Do.
CsF	75·9	(184)	$0{\cdot}050_5$	$0{\cdot}22_5$	Do.
CsI	129·9	(95)	0·109	0·33	Do.
AgCl	71·67	130	0·092	$0{\cdot}30_5$	Θ from limit of T^3/C_v (Clusius & Harteck, 1928)
AgI	117·4	120	0·076	$0{\cdot}27_5$	Do.
LiH	3·975	815	$0{\cdot}058_5$	0·24	Ubbelohde (1936)
LiD	4·475	611	$0{\cdot}085_5$	0·29	Do.
PbS	119·7	~ 190	0·030	$0{\cdot}17_5$	Θ from limit of T^3/C_v
ZnS	48·72	265	$0{\cdot}038_5$	$0{\cdot}19_5$	Clusius & Harteck (1928)
(zincblende)		230	$0{\cdot}050_5$	$0{\cdot}22_5$	Günther (1916)
FeS_2	39·99	645	0·013	0·11	Seitz, from specific heats
CaF_2	26·03	474	$0{\cdot}014_5$	0·12	Do.
$NaClO_3$	21·29	~ 850	0·010	0·10	Approx. value of Θ by analogy with orthorhombic $KClO_3$ and with other Na and K compounds

It may be noted that an error of say 10% in the value of Θ would lead to an error in $\sqrt{(\overline{u^2})}$ of about the same magnitude but of opposite sign. The data for $NaClO_3$ are given because of the analogy between its structure and that of ZnS, and because of the practical interest of both substances, but the value of Θ given is questionable. It should not be difficult, and would be very interesting, to measure $\sqrt{(\overline{u^2})}$ for $NaClO_3$ by X-ray methods, and to see whether the value given in Table 3 is of the correct order of magnitude. Two values of Θ are given for zincblende because the experimental data are conflicting. (The values of specific heats given in the *International Critical Tables* appear to be in disagreement with both sources quoted above and would give a much lower value of Θ altogether; on the other hand, Försterling (1921) deduces from the elastic constants of Voigt (1918) a value which is higher than either of those given here.) Here again a measurement of $\sqrt{(\overline{u^2})}$ by X-ray methods would be valuable, as also in the case of AgCl, where the value of Θ given by Seitz is inconsistent with the specific heat data of Clusius & Harteck (1928).

2. Spatial distribution of atomic displacements

It has long been known that the thermal vibrations are not really isotropic, even in monatomic cubic crystals (Born & v. Kármán, 1912). A measurement of the amplitudes of waves of different polarizations having different directions of propagation may be made by studying the intensity of diffuse X-ray scattering in the neighbourhood of the Bragg reflexions (Laval, 1935, 1939). In the case of a harmonic vibration in which the atomic movements are normal to a given set of crystal planes there is a resulting change of intensity of reflecting power which is, to a first approximation, proportional to the mean-square amplitude of the oscillation. This change in intensity causes a reduction of the Bragg reflexion, but the energy reappears as diffuse scattering. Measurements of the change of *Bragg* reflexion give an integrated effect and do not distinguish the different effects of different types of vibrations, but measurements of *diffuse* scattering, if properly made (with a narrow, parallel monochromatic beam and a stationary crystal, for different orientations) make just this distinction. Jahn (1942) has given a simple derivation of the relative intensities of diffuse thermal scattering in different directions around reciprocal lattice points for a cubic crystal, in terms of the elastic constants c_{11}, c_{12} and c_{44}; and good qualitative agreement has been obtained experimentally for Na, Pb, W, NaCl and KCl (Lonsdale & Smith, 1942; Lonsdale, 1942, 1943). That is to say, the shapes of the isodiffusion surfaces in the neighbourhood of reciprocal lattice points which are found experimentally are just those given by the Jahn formula

$$
\begin{aligned}
I \propto \frac{R^2}{r^2}\{c_{44}^2 + \Sigma L^2[c_{44}(c_{11}-c_{44})\,(m^2+n^2) \\
+ (c_{11}+c_{12})\,(c_{11}-c_{12}-2c_{44})\,m^2n^2] \\
-2\Sigma MNmn(c_{12}+c_{44})\,[c_{44}+(c_{11}-c_{12}-2c_{44})\,l^2]\} \\
\div\{c_{11}c_{44}^2 + c_{44}(c_{11}+c_{12})\,(c_{11}-c_{12}-2c_{44}) \\
\times (m^2n^2+n^2l^2+l^2m^2) \\
+ (c_{11}+2c_{12}+c_{44})\,(c_{11}-c_{12}-2c_{44})^2\,l^2m^2n^2\}. \qquad (4)
\end{aligned}
$$

Here I is the intensity of diffuse reflecting power at a (small) distance r and in the direction $[uvw]$ (having direction cosines l, m, n) from the reciprocal-lattice point hkl. The distance of this point from the origin of reciprocal space is R in a direction defined by the direction cosines L, M, N. (I.e. $l = u/\surd(u^2+v^2+w^2)$, etc.; $L = h/\surd(h^2+k^2+l^2)$, etc.) As Jahn has shown, the substitution of particular values of l, m, n, L, M, N can simplify this formula considerably. In fact, along particular directions it represents the effect of a pure transverse or a pure longitudinal wave (with a frequency directly proportional to r), having its amplitude normal to a main crystal plane.

For instance, if we consider the reciprocal lattice point 001 and the direction [100] ($L = M = 0$, $N = 1$; $l = 1$, $m = n = 0$), then expression (4) becomes

$$I \propto \frac{R^2}{r^2}\frac{1}{c_{44}}.$$

Here we are considering the effect of a pure transverse wave whose direction of propagation is [100], whose amplitude is normal to the set of planes (001), and whose velocity in a crystal of density ρ is $\surd(c_{44}/\rho)$. Now the mean-square displacement, $\overline{\xi^2}$, corresponding to waves of this class, must be proportional to $1/c_{44}$, since $I \propto \overline{\xi^2}$, at least to a first approximation, for waves of relatively low frequency (small r-value).

For the reciprocal-lattice point 001 and the direction [001], the expression (4) represents the effect of a pure longitudinal wave, velocity $\surd(c_{11}/\rho)$, and of mean-square displacement proportional to $1/c_{11}$ for low-frequency waves.

If we use the following abbreviations

$$a = \frac{1}{c_{11}}, \quad b = \frac{1}{c_{44}}, \quad c = \frac{1}{c_{11}-c_{12}}, \quad d = \frac{1}{c_{11}+c_{12}+2c_{44}},$$

$$e = \frac{1}{c_{11}+2c_{12}+4c_{44}}, \quad f = \frac{1}{c_{11}-c_{12}+c_{44}},$$

then a, d and e are proportional to the mean-square displacement $\overline{\xi^2}$ for pure longitudinal waves and b, c, f are proportional to the mean-square displacement $\overline{\xi^2}$ for pure transverse waves. Jahn's formula can be applied to give relative values of the mean-square displacement normal to the set of planes (hkl) due to all waves whose direction of propagation is [uvw]. Special cases are given in Table 4.

If for any particular crystal the measured values of c_{11}, c_{12} and c_{44} are substituted in the above, the spatial distribution of root-mean square amplitudes, $\surd(\overline{\xi^2})$, for waves of different polarizations travelling in different directions may be found for any given frequency

Table 4. *Intensity of diffuse reflecting power; varying mean-square displacement.*
(*Special cases of Jahn's formula; r constant*)

$[uvw]$	(hkl)	(001)	(110)	(210)	(111)	(112)
[100]	$L^2a+(M^2+N^2)\,b$	b	$\frac{1}{2}(a+b)$	$\frac{1}{5}(4a+b)$	$\frac{1}{3}(a+2b)$	$\frac{1}{6}(a+5b)$
[010]	$M^2a+(N^2+L^2)\,b$	b	$\frac{1}{2}(a+b)$	$\frac{1}{5}(a+4b)$	$\frac{1}{3}(a+2b)$	$\frac{1}{6}(a+5b)$
[001]	$N^2a+(L^2+M^2)\,b$	a	b	b	$\frac{1}{3}(a+2b)$	$\frac{1}{3}(2a+b)$
[110]	$(L+M)^2\,d+(L-M)^2\,c+N^2b$	b	$2d$	$\frac{1}{5}(9d+c)$	$\frac{1}{3}(b+4d)$	$\frac{1}{3}(2d+2b)$
[101]	$(N+L)^2\,d+(N-L)^2\,c+M^2b$	$c+d$	$\frac{1}{2}(b+c+d)$	$\frac{1}{5}(4d+4c+b)$	$\frac{1}{3}(b+4d)$	$\frac{1}{6}(9d+c+b)$
[011]	$(M+N)^2\,d+(M-N)^2\,c+L^2b$	$c+d$	$\frac{1}{2}(b+c+d)$	$\frac{1}{5}(d+c+4b)$	$\frac{1}{3}(b+4d)$	$\frac{1}{6}(9d+c+b)$
$[\bar{1}10]$	$(L-M)^2\,d+(L+M)^2\,c+N^2b$	b	$2c$	$\frac{1}{5}(d+9c)$	$\frac{1}{3}(b+4c)$	$\frac{1}{3}(2c+2b)$
$[10\bar{1}]$	$(N-L)^2\,d+(N+L)^2\,c+M^2b$	$c+d$	$\frac{1}{2}(b+c+d)$	$\frac{1}{5}(4d+4c+b)$	$\frac{1}{3}(b+4c)$	$\frac{1}{6}(d+9c+b)$
$[0\bar{1}1]$	$(M-N)^2\,d+(M+N)^2\,c+L^2b$	$c+d$	$\frac{1}{2}(b+c+d)$	$\frac{1}{5}(d+c+4b)$	$\frac{1}{3}(b+4c)$	$\frac{1}{6}(d+9c+b)$
[111]	$(L+M+N)^2\,e+2(1-LM-MN-NL)\,f$	$c+2f$	$2e+f$	$\frac{1}{5}(9e+6f)$	$3e$	$\frac{1}{3}(8e+f)$
$[\bar{1}11]$	$(-L+M+N)^2\,e+2(1+LM-MN+NL)\,f$	$e+2f$	$2e+f$	$\frac{1}{5}(9e+6f)$	$\frac{1}{3}(e+8f)$	$3f$
$[1\bar{1}1]$	$(L-M+N)^2\,e+2(1+LM+MN-NL)\,f$	$e+2f$	$3f$	$\frac{1}{5}(e+14f)$	$\frac{1}{3}(e+8f)$	$\frac{1}{3}(2e+7f)$
$[11\bar{1}]$	$(L+M-N)^2\,e+2(1-LM+MN+NL)\,f$	$e+2f$	$3f$	$\frac{1}{5}(e+14f)$	$\frac{1}{3}(e+8f)$	$\frac{1}{3}(2e+7f)$

Sum: $\Sigma L^2(a+4b+4c+4d+4c+8f) = a+4(b+c+d+e)+8f$

(r constant); but it will be seen that although this distribution varies considerably from one reciprocal point to another, and has a wide range in respect of any one lattice point (variations of as much as 14 to 1 exist, for instance, in the Na crystal), yet the value of $\Sigma\overline{\xi^2}$, summed over all the wave directions given, is constant for all reciprocal-lattice points, as it should be for a cubic crystal. In the case of the thirteen wave directions considered in Table 4, $\Sigma\overline{\xi^2}\propto a+4(b+c+d+e)+8f$. A different sum would, of course, be obtained if other directions were also considered, but it would be constant for all reciprocal-lattice points provided that all crystallographically equivalent directions were included in the summation. This result follows from the fact that the mean-square amplitude of all vibrations taken together is the same in any direction in the crystal, so that M may be calculated from intensity measurements made on any set of planes in a monatomic cubic crystal, in spite of the fact that the *distribution* of values of $\overline{\xi^2}$ going to make up $\overline{u_x^2}(=\frac{1}{3}\overline{u^2})$ varies with direction. Jahn's formula, as has been mentioned previously, gives only relative values of $\overline{\xi^2}$ for waves of low frequency (that is, frequencies which satisfy the relation $h\nu\ll kT$). For such waves $\overline{\xi^2}\sim\frac{1}{2}kT$, and since ν may vary from zero to a limiting value (Born & v. Kármán, 1912; Kellermann, 1940, 1941; Iona, 1941), it follows that $\overline{\xi^2}$ may, in fact, be very large for the low-frequency waves, a fact which explains the comparatively high intensity of diffuse scattering near to the Bragg reflexion positions at least in certain directions. For high-frequency waves (ν large)

$$\overline{\xi^2}\sim\frac{h}{2\nu}\left(\frac{e^{\beta}+1}{e^{\beta}-1}\right),$$

where $\beta=h\nu/kT$, and in the region of the maxima of the frequency spectrum $\overline{\xi^2}$ will be more nearly proportional to $1/\nu$ (i.e. to the square roots of the values given in Table 4); but the same general distribution law as that given in Table 4 appears to hold, according to the X-ray experimental evidence, for a considerable distance around each reciprocal lattice point (that is, for a considerable range of frequencies).

The amount of experimental data recorded for the elastic constants of cubic crystals is limited. Table 5 gives the room temperature values available.

Table 5. *Elastic constants of cubic crystals*

(Unit: 10^{11} dynes cm.$^{-2}$)

Substance	c_{11}	c_{12}	c_{44}	Remarks and references
Pb	4·77	4·03	1·44	Goens (corrected) (1936)
Al	10·8	6·2	2·8	Schmid & Boas (1935)
Ag	12·0	8·97	4·36	Do.
Au	19·4	16·6	4·0	Do.
Cu	17·0	12·3	7·53	Do.
Na	0·52	0·40	0·41	Extrapolated from Quimby & Siegel (1938)
α-Fe	23·7	14·1	11·6	Schmid & Boas (1935)
W	51·3	20·6	15·3	Do.
C (diamond)	95·0	39	43	Bhagavantam & Suryanarayan (1944)
NaCl	4·97	1·27	1·27	Bhagavantam (1946)
NaBr	3·30	1·31	1·33	Schmid & Boas (1935)
KCl	3·70	0·81	0·79	Do.
KBr	3·33	0·58	0·62	Do.
KI	2·67	0·43	0·42	Do.
PbS	8·69	4·01	4·42	Bhagavantam (1946)
ZnS	10·79	7·22	4·12	Bhagavantam & Suryanarayan (1944)
FeS_2	36·3	−4·7	10·5	Doraiswami (1947)
CaF_2	16·44	5·02	3·47	Bhagavantam (1946)
$NaClO_3$ (1)	6·19	−2·09	1·20	Voigt (1910)
(2)	5·09	1·55	1·18	Bhagavantam & Suryanarayan (1947)
(3)	4·90	1·39	1·17	Mason (1946)

Of all these substances only tungsten is elastically isotropic ($c_{11}-c_{12}=2c_{44}$), but even for this crystal the values of $\overline{\xi^2}$ for different types of vibration vary over a range of more than three to one. The mean-square amplitudes of the longitudinal waves, in any direction of propagation, are invariably small relative to those of transverse waves of the same frequency. It is clearly not possible to give absolute values of corresponding atomic displacements, $\sqrt{(\overline{\xi^2})}$, without specifying the range of frequency covered and without knowing the distribution in the frequency spectrum, but in order to relate the values of the individual wave amplitudes to the mean-square amplitude of vibration $\overline{u^2}$ for the different crystals, relative values of $\sqrt{(\overline{\xi^2})}$ are given in terms of $(\Sigma\overline{\xi^2})=13\overline{u^2}$, summing over the thirteen wave directions of Table 4. It must be clearly understood, however, that these values have no absolute significance, though they have a relative significance not only for each crystal but from one crystal to another. So also have the values of the intensity of diffuse scattering I, which are proportional to $\overline{\xi^2}$ at any given r value. Table 6 gives a complete range of values for a few typical crystals, together with $\sqrt{(\overline{u^2})}$ values and 1st, 2nd and 3rd nearest neighbour distances; while Table 7 gives relative values of $\sqrt{(\overline{\xi^2})}$ for the pure longitudinal and pure transverse waves for all crystals listed in Table 5.

Table 6. *Relative values of intensity of diffuse scattering and of root mean-square atomic displacements*

(Displacements in true A. using the relation 1 kX. = 1·00202 A.)

Pb (A1 type): $\sqrt{(\overline{u^2})} = 0{\cdot}28$ A.; Pb_0–Pb_1 = 3·50; Pb_0–Pb_2 = 4·95; Pb_0–Pb_3 = 6·06 A.

	$I \sim \overline{\xi^2}$					$\sqrt{(\overline{\xi^2})}$				
	(001)	(110)	(210)	(111)	(112)	(001)	(110)	(210)	(111)	(112)
[100]	5·3	$3{\cdot}4_5$	$2{\cdot}3_5$	$4{\cdot}0_5$	$4{\cdot}7 \times 10^{-2}$	0·23	$0{\cdot}18_5$	0·15	0·20	0·22
[010]	5·3	$3{\cdot}4_5$	$4{\cdot}5_5$	$4{\cdot}0_5$	4·7	0·23	$0{\cdot}18_5$	0·21	0·20	0·22
[001]	1·6	5·3	5·3	$4{\cdot}0_5$	2·8	0·13	0·23	0·23	0·20	0·17
[110]	5·3	1·3	$3{\cdot}5_5$	$2{\cdot}6_5$	4·0	0·23	0·11	0·19	0·16	0·20
[101]	12·6	8·9	11·1	$2{\cdot}6_5$	$3{\cdot}8_5$	$0{\cdot}35_5$	0·30	0·33	0·16	$0{\cdot}19_5$
[011]	12·6	8·9	3·7	$2{\cdot}6_5$	$3{\cdot}8_5$	$0{\cdot}35_5$	0·30	0·19	0·16	$0{\cdot}19_5$
$[\bar{1}10]$	5·3	23·8	$21{\cdot}5_5$	$17{\cdot}6_5$	11·4	0·23	0·49	$0{\cdot}46_5$	0·42	0·34
$[10\bar{1}]$	12·6	8·9	11·1	$17{\cdot}6_5$	$18{\cdot}8_5$	$0{\cdot}35_5$	0·30	0·33	0·42	$0{\cdot}43_5$
$[0\bar{1}1]$	12·6	8·9	3·7	$17{\cdot}6_5$	$18{\cdot}8_5$	$0{\cdot}35_5$	0·30	0·19	0·42	$0{\cdot}43_5$
[111]	$7{\cdot}7_5$	4·5	5·1	$1{\cdot}2_5$	2·3	0·28	0·21	$0{\cdot}22_5$	0·11	0·15
$[\bar{1}11]$	$7{\cdot}7_5$	4·5	5·1	9·9	11·0	0·28	0·21	$0{\cdot}22_5$	$0{\cdot}31_5$	0·33
$[1\bar{1}1]$	$7{\cdot}7_5$	4·5	$10{\cdot}3_5$	9·9	8·8	0·28	0·21	0·32	$0{\cdot}31_5$	0·30
$[11\bar{1}]$	$7{\cdot}7_5$	4·5	$10{\cdot}3_5$	9·9	8·8	0·28	0·21	0·32	$0{\cdot}31_5$	0·30

W (A2 type): $\sqrt{(\overline{u^2})} = 0{\cdot}086$ A.; W_0–W_1 = 2·74; W_0–W_2 = $3{\cdot}16_5$; W_0–W_3 = 4·48 A.

	$I \sim \overline{\xi^2}$					$\sqrt{(\overline{\xi^2})}$				
	(001)	(110)	(210)	(111)	(112)	(001)	(110)	(210)	(111)	(112)
[100]	1·0	$0{\cdot}6_5$	$0{\cdot}4_5$	$0{\cdot}7_5$	$0{\cdot}9 \times 10^{-2}$	0·10	0·08	0·07	$0{\cdot}08_5$	$0{\cdot}09_5$
[010]	1·0	$0{\cdot}6_5$	$0{\cdot}8_5$	$0{\cdot}7_5$	0·9	0·10	0·08	0·09	$0{\cdot}08_5$	$0{\cdot}09_5$
[001]	0·3	1·0	1·0	$0{\cdot}7_5$	0·5	$0{\cdot}05_5$	0·10	0·10	$0{\cdot}08_5$	0·07
[110]	1·0	0·3	$0{\cdot}3_5$	0·5	$0{\cdot}7_5$	0·10	$0{\cdot}05_5$	0·06	0·07	$0{\cdot}08_5$
[101]	$0{\cdot}6_5$	0·8	0·7	0·5	$0{\cdot}4_5$	0·08	0·09	$0{\cdot}08_5$	0·07	0·07
[011]	$0{\cdot}6_5$	0·8	0·9	0·5	$0{\cdot}4_5$	0·08	0·09	$0{\cdot}09_5$	0·07	0·07
$[\bar{1}10]$	1·0	1·0	0·9	1·0	1·0	0·10	0·10	$0{\cdot}09_5$	0·10	0·10
$[10\bar{1}]$	$0{\cdot}6_5$	0·8	0·7	1·0	0·9	0·08	0·09	0·08	0·10	$0{\cdot}09_5$
$[0\bar{1}1]$	$0{\cdot}6_5$	0·8	0·9	1·0	0·9	0·08	0·09	$0{\cdot}09_5$	0·10	$0{\cdot}09_5$
[111]	$0{\cdot}7_5$	0·5	0·6	0·3	0·4	$0{\cdot}08_5$	0·07	0·08	$0{\cdot}05_5$	$0{\cdot}06_5$
$[\bar{1}11]$	$0{\cdot}7_5$	0·5	0·6	0·9	1·0	$0{\cdot}08_5$	0·07	0·08	$0{\cdot}09_5$	0·10
$[1\bar{1}1]$	$0{\cdot}7_5$	1·0	0·9	0·9	0·8	$0{\cdot}08_5$	0·10	$0{\cdot}09_5$	$0{\cdot}09_5$	0·09
$[11\bar{1}]$	$0{\cdot}7_5$	1·0	0·9	0·9	0·8	$0{\cdot}08_5$	0·10	$0{\cdot}09_5$	$0{\cdot}09_5$	0·09

KI (B1 type): $\sqrt{(\overline{u^2})} = 0{\cdot}30_5$ A.; K_0–I_0 = 3·53; K_0–K_1 = 5·00; K_0–I_1 = 6·12 A.

	$I \sim \overline{\xi^2}$					$\sqrt{(\overline{\xi^2})}$				
	(001)	(110)	(210)	(111)	(112)	(001)	(110)	(210)	(111)	(112)
[100]	17·5	10·1	5·7	12·6	$15{\cdot}0 \times 10^{-2}$	0·42	0·32	0·24	$0{\cdot}35_5$	0·39
[010]	17·5	10·1	14·5	12·6	15·0	0·42	0·32	0·38	$0{\cdot}35_5$	0·39
[001]	$2{\cdot}7_5$	17·5	17·5	12·6	$7{\cdot}6_5$	$0{\cdot}16_5$	0·42	0·42	$0{\cdot}35_5$	$0{\cdot}27_5$
[110]	17·5	3·7	4·0	8·3	12·8	0·42	$0{\cdot}19_5$	0·20	0·29	0·36
[101]	$5{\cdot}1_5$	11·3	7·6	8·3	$6{\cdot}2_5$	$0{\cdot}22_5$	$0{\cdot}33_5$	$0{\cdot}27_5$	0·29	0·25
[011]	$5{\cdot}1_5$	11·3	15·0	8·3	$6{\cdot}2_5$	$0{\cdot}22_5$	$0{\cdot}33_5$	0·39	0·29	0·25
[110]	17·5	$6{\cdot}5_5$	$6{\cdot}2_5$	10·2	$13{\cdot}8_5$	0·42	$0{\cdot}25_5$	$0{\cdot}25_5$	0·32	0·37
$[10\bar{1}]$	$5{\cdot}1_5$	11·3	7·6	10·2	$8{\cdot}1_5$	$0{\cdot}22_5$	$0{\cdot}33_5$	$0{\cdot}27_5$	0·32	$0{\cdot}28_5$
$[0\bar{1}1]$	$5{\cdot}1_5$	11·3	15·0	10·2	$8{\cdot}1_5$	$0{\cdot}22_5$	$0{\cdot}33_5$	0·39	0·32	$0{\cdot}28_5$
[111]	6·9	5·6	$5{\cdot}8_5$	4·2	4·7	0·26	$0{\cdot}23_5$	0·24	$0{\cdot}20_5$	0·22
$[\bar{1}11]$	6·9	5·6	$5{\cdot}8_5$	7·8	8·3	0·26	$0{\cdot}23_5$	0·24	0·28	0·29
$[1\bar{1}1]$	6·9	8·3	8·0	7·8	7·4	0·26	0·29	0·28	0·28	0·27
[111]	6·9	8·3	8·0	7·8	7·4	0·26	0·29	0·28	0·28	0·27

ZnS (B2 type): $\sqrt{(\overline{u^2})} = 0{\cdot}19_5$ A.; Zn_0–S_0 = 2·35; Zn_0–Zn_1 = 3·84; Zn_0–S_1 = 4·50 A.

(The following values are referred to the Clusius-Harteck specific heat data.)

	$I \sim \overline{\xi^2}$					$\sqrt{(\xi^2)}$				
	(001)	(110)	(210)	(111)	(112)	(001)	(110)	(210)	(111)	(112)
[100]	3·5	2·4	1·75	$2{\cdot}7_5$	$3{\cdot}1 \times 10^{-2}$	$0{\cdot}18_5$	$0{\cdot}15_5$	0·13	$0{\cdot}16_5$	$0{\cdot}17_5$
[010]	3·5	2·4	$3{\cdot}0_5$	$2{\cdot}7_5$	3·1	$0{\cdot}18_5$	$0{\cdot}15_5$	$0{\cdot}17_5$	$0{\cdot}16_5$	$0{\cdot}17_5$
[001]	1·3	3·5	3·5	$2{\cdot}7_5$	$2{\cdot}0_5$	$0{\cdot}11_5$	$0{\cdot}18_5$	$0{\cdot}18_5$	$0{\cdot}16_5$	$0{\cdot}14_5$
[110]	3·5	1·1	1·8	1·9	2·7	$0{\cdot}18_5$	$0{\cdot}10_5$	$0{\cdot}13_5$	0·14	$0{\cdot}16_5$
[101]	$4{\cdot}5_5$	4·0	$4{\cdot}3_5$	1·9	2·1	$0{\cdot}21_5$	0·20	0·21	0·14	$0{\cdot}14_5$
[011]	$4{\cdot}5_5$	4·0	3·7	1·9	2·1	$0{\cdot}21_5$	0·20	0·19	0·14	$0{\cdot}14_5$
$[\bar{1}10]$	3·5	$8{\cdot}0_5$	$7{\cdot}3_5$	6·5	5·0	$0{\cdot}18_5$	$0{\cdot}28_5$	0·27	$0{\cdot}25_5$	$0{\cdot}22_5$
$[10\bar{1}]$	$4{\cdot}5_5$	4·0	$4{\cdot}3_5$	6·5	6·7	$0{\cdot}21_5$	0·20	0·21	$0{\cdot}25_5$	0·26
$[0\bar{1}1]$	$4{\cdot}5_5$	4·0	3·7	6·5	6·7	$0{\cdot}21_5$	0·20	0·19	$0{\cdot}25_5$	0·26
[111]	4·1	$2{\cdot}5_5$	$2{\cdot}8_5$	1·0	$1{\cdot}5_5$	0·20	0·16	0·17	0·10	$0{\cdot}12_5$
$[\bar{1}11]$	4·1	$2{\cdot}5_5$	$2{\cdot}8_5$	5·1	5·6	0·20	0·16	0·17	$0{\cdot}22_5$	$0{\cdot}23_5$
$[1\bar{1}1]$	4·1	5·6	5·3	5·1	4·6	0·20	$0{\cdot}23_5$	0·23	$0{\cdot}22_5$	$0{\cdot}21_5$
$[11\bar{1}]$	4·1	5·6	5·3	5·1	4·6	0·20	$0{\cdot}23_5$	0·23	$0{\cdot}22_5$	$0{\cdot}21_5$

Table 6 (*cont.*)

FeS_2 (C2 type): $\sqrt{(\overline{u^2})} = 0{\cdot}11$ A.; S_0–$S_1 = 2{\cdot}10$; S_0–$Fe_0 = 2{\cdot}26$; S_0–$S_2 = 3{\cdot}10$ A.

	$I \sim \overline{\xi^2}$					$\sqrt{(\overline{\xi^2})}$				
	(001)	(110)	(210)	(111)	(112)	(001)	(110)	(210)	(111)	(112)
[100]	2·0	1·3	$0{\cdot}8_5$	1·5	$1{\cdot}7_5 \times 10^{-2}$	0·14	$0{\cdot}11_5$	0·09	0·12	0·13
[010]	2·0	1·3	1·7	1·5	$1{\cdot}7_5$	0·14	$0{\cdot}11_5$	0·13	0·12	0·13
[001]	$0{\cdot}5_5$	2·0	2·0	1·5	$1{\cdot}0_5$	$0{\cdot}07_5$	0·14	0·14	0·12	0·10
[110]	2·0	0·8	0·8	1·2	1·6	0·14	0·09	0·09	0·11	$0{\cdot}12_5$
[101]	0·9	$1{\cdot}4_5$	1·1	1·2	1·0	$0{\cdot}09_5$	0·12	$0{\cdot}10_5$	0·11	0·10
[011]	0·9	$1{\cdot}4_5$	1·8	1·2	1·0	$0{\cdot}09_5$	0·12	$0{\cdot}13_5$	0·11	0·10
$[\bar{1}10]$	2·0	1·0	1·0	$1{\cdot}3_5$	1·7	0·14	0·10	0·10	$0{\cdot}11_5$	0·13
$[10\bar{1}]$	0·9	$1{\cdot}4_5$	1·1	$1{\cdot}3_5$	$1{\cdot}1_5$	$0{\cdot}09_5$	0·12	$0{\cdot}10_5$	$0{\cdot}11_5$	$0{\cdot}10_5$
$[0\bar{1}1]$	0·9	$1{\cdot}4_5$	1·8	$1{\cdot}3_5$	$1{\cdot}1_5$	$0{\cdot}09_5$	0·12	$0{\cdot}13_5$	$0{\cdot}11_5$	$0{\cdot}10_5$
[111]	1·1	1·0	$1{\cdot}0_5$	0·9	$0{\cdot}9_5$	$0{\cdot}10_5$	0·10	0·10	$0{\cdot}09_5$	$0{\cdot}09_5$
$[\bar{1}11]$	1·1	1·0	$1{\cdot}0_5$	1·2	1·2	$0{\cdot}10_5$	0·10	0·10	0·11	0·11
$[1\bar{1}1]$	1·1	1·2	1·2	1·2	$1{\cdot}1_5$	$0{\cdot}10_5$	0·11	0·11	0·11	$0{\cdot}10_5$
$[11\bar{1}]$	1·1	1·2	1·2	1·2	$1{\cdot}1_5$	$0{\cdot}10_5$	0·11	0·11	0·11	$0{\cdot}10_5$

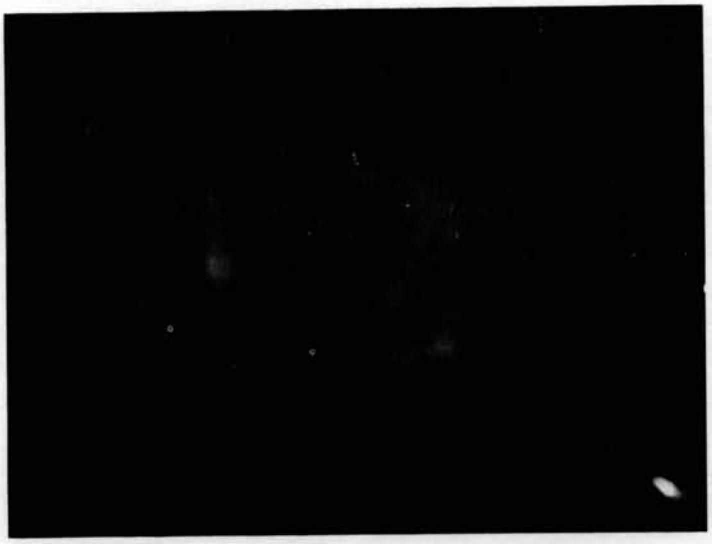
Table 7. *Relative root mean-square atomic displacements corresponding to pure longitudinal and transverse waves.*

(Lattice constants and displacements are given in true A.; $\sqrt{a}$ etc. are given in terms of $a + 4(b + c + d + e) + 8f = 13\overline{u^2}$.)

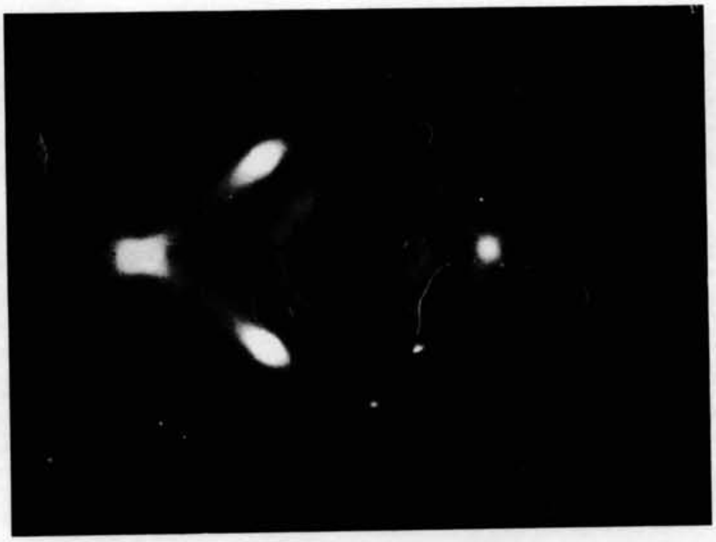
	Structure type	Lattice constant	$\sqrt{(\overline{u^2})}$	Longitudinal $\sqrt{(\overline{\xi^2})}$			Transverse $\sqrt{(\overline{\xi^2})}$		
				$\sqrt{a}$	$\sqrt{(2d)}$	$\sqrt{(3e)}$	$\sqrt{b}$	$\sqrt{(2c)}$	$\sqrt{(3f)}$
Pb	A1	4·949	0·28	0·13	0·11	0·11	0·23	0·49	0·33
Al	A1	4·049	0·18	0·10	0·10	0·10	0·20	0·22	$0{\cdot}21_5$
Ag	A1	4·086	0·16	0·09	0·08	$0{\cdot}07_5$	$0{\cdot}14_5$	0·25	$0{\cdot}19_5$
Au	A1	4·078	0·15	$0{\cdot}06_5$	0·06	0·06	0·14	$0{\cdot}23_5$	$0{\cdot}18_5$
Cu	A1	3·615	$0{\cdot}14_5$	$0{\cdot}08_5$	$0{\cdot}07_5$	0·07	$0{\cdot}12_5$	0·23	$0{\cdot}17_5$
Na	A2	4·290	0·50	0·31	0·24	$0{\cdot}22_5$	0·35	0·92	$0{\cdot}53_5$
α-Fe	A2	2·865	$0{\cdot}11_5$	$0{\cdot}07_5$	0·07	$0{\cdot}06_5$	0·11	0·17	0·14
W	A2	3·165	$0{\cdot}08_5$	$0{\cdot}05_5$	$0{\cdot}05_5$	$0{\cdot}05_5$	0·10	0·10	0·10
C (diamond)	A4	3·567	0·02	$0{\cdot}01_5$	$0{\cdot}01_5$	$0{\cdot}01_5$	0·02	$0{\cdot}02_5$	$0{\cdot}02_5$
NaCl	B1	5·639	0·24	$0{\cdot}14_5$	$0{\cdot}15_5$	0·16	0·29	0·24	$0{\cdot}25_5$
NaBr	B1	5·971	0·25	0·17	0·16	$0{\cdot}18_5$	0·27	0·31	$0{\cdot}29_5$
KCl	B1	6·290	0·26	$0{\cdot}15_5$	0·17	$0{\cdot}17_5$	$0{\cdot}33_5$	$0{\cdot}24_5$	$0{\cdot}26_5$
KBr	B1	6·599	$0{\cdot}26_5$	0·15	0·17	0·18	0·35	$0{\cdot}23_5$	0·26
KI	B1	7·066	$0{\cdot}30_5$	$0{\cdot}16_5$	$0{\cdot}19_5$	$0{\cdot}20_5$	0·42	$0{\cdot}25_5$	0·29
PbS	B1	5·98	$0{\cdot}17_5$	0·12	0·11	$0{\cdot}10_5$	0·17	$0{\cdot}23_5$	$0{\cdot}20_5$
ZnS	B3	5·44	$0{\cdot}19_5$	$0{\cdot}11_5$	$0{\cdot}10_5$	0·10	$0{\cdot}18_5$	$0{\cdot}28_5$	$0{\cdot}23_5$
FeS_2	C2	5·424	0·11	$0{\cdot}07_5$	0·09	$0{\cdot}09_5$	0·14	0·10	0·11
CaF_2	C1	5·47	0·12	0·07	$0{\cdot}07_5$	0·08	$0{\cdot}15_5$	$0{\cdot}11_5$	$0{\cdot}12_5$
$NaClO_3$	G3	$6{\cdot}58_3$	0·10	(1) 0·06 (2) 0·06	0·08 $0{\cdot}06_5$	$0{\cdot}09_5$ $0{\cdot}06_5$	$0{\cdot}13_5$ $0{\cdot}12_5$	0·07 0·10	0·08 0·11

In Table 7, $\sqrt{a}$ represents the effect of a pure longitudinal wave travelling along a cube edge, $\sqrt{(2d)}$ that of one along a face diagonal, $\sqrt{(3e)}$ that of one along a cube diagonal. In general there is little difference in the relative amplitudes of these vibrations, although it may be seen that for the metals (whether face-centred, A1, or body-centred, A2) the largest amplitudes (smallest velocities for a given frequency) are associated with the cube edges, presumably because the atoms are farthest apart along these directions. For the rock-salt type of compounds (with the exception of NaBr and PbS) just the reverse conditions apply, and again the slow, large amplitude wave is associated with the direction of largest atomic separation, now along [111]. The same general rule applies to ZnS and FeS_2.

For the doubly degenerate pure transverse waves, $\sqrt{b}$, $\sqrt{(2c)}$ and $\sqrt{(3f)}$ are again associated with the cube edge, the face diagonal and the cube diagonal respectively, as directions of propagation, the displacements being in any two mutually perpendicular directions at right angles to these directions. Here there is a more distinct difference, in general, between the different directions, and also between the behaviour of the metals and that of the rock-salt type structures. In the case of the metals, the slowest pure transverse waves are those along the face diagonals (whether the structure is body-centred or face-centred), and these therefore have the largest relative amplitudes. In the case of Na in particular, the amplitudes of such waves are very large indeed, and the existence of *continuous* diffuse scattering streaks along the corresponding diagonal directions in reciprocal space (see Plate 6) shows that this is true even when the waves are of such high frequency that they correspond to wave-lengths comparable with the interatomic distances. The large amplitudes of atomic vibration in sodium may well explain the self-annealing effects observed as an intensity hysteresis by Dawton (1937) during repeated cycles of heating and cooling. That similar data would apply for Li is clear, not only from the similarity of their



Sodium single crystal in thin glass tube. [$1\bar{1}0$] axis vertical. Monochromatized Cu $K\alpha$ radiation (urea nitrate monochromator) at angle $\theta_B + 5°$ to plane (110). All streaks correspond to various [$1\bar{1}0$] directions. Room temperature. Exposure time 2 hr.



Sodium single crystal in thin glass tube. [100] axis vertical. Monochromatized Cu $K\alpha$ radiation at correct Bragg angle for 002 reflexion. Streaks along [110] directions. The inner diffraction ring is due to the glass tube. Room temperature. Exposure time 1 hr.

atomic and crystal structure but from the similarity of their diffuse scattering patterns. It is because of these large dynamic displacements normal to the (110) planes that Barrett (1947) was able, by suitable cold-working at temperatures below −196° C., to cause a transformation of Li from its usual body-centred cubic structure to a face-centred structure.

For the rock-salt type of structure, however (again with the exception of NaBr and PbS), the slowest transverse waves are those along the cube edges. In other words, it is difficult for ions of opposite sign to vary their relative distance along their line of closest approach, but relatively easy for them to vibrate about this line. This leads to a streaking of diffuse scattering along the cube directions in reciprocal space (other than those which pass through the origin), which should be particularly well marked in the case of KI. The tendency to vibrate about the line of closest approach is least in the case of like ions. For KI, indeed, such transverse vibrations (wave propagation along face diagonals) have amplitudes only a little bigger than those of the longitudinal waves travelling in the same direction. There is an interesting tendency for ZnS and PbS to behave like the metals, whereas FeS_2, CaF_2 and $NaClO_3$ are more like the alkali halides in their elastic behaviour. This is confirmed for $NaClO_3$ by the recent paper of Garrido (1948) giving a qualitative account of the diffuse scattering of that substance. A more precise quantitative measurement of the diffuse scattering should certainly be able to distinguish between elastic data as diverse as those of Voigt and of Bhagavantam & Suryanarayan, since the former would give much more anisotropic effects; but the method would be unlikely to distinguish between the latter's data and those of Mason (see Table 5).

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