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Theory of the Photoelastic Effect of Cubic Crystals

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The theory of Ewald and Born of the double refraction of crystals is applied to the calculation of the photoelastic properties of D lattices. Only in special cases, as for instance in KCl for pressure parallel [111], is the effect determined by the anisotropy of the Lorentz and Coulomb forces. In these cases the photoelastic data determine the ratio $R_{\text{Cl}}/R_{\text{K}}$ of the ionic refractions. Satisfactory agreement with all observations can be reached by assuming that the elastic deformations produce optical anisotropy of the atoms. Introducing this assumption in the Ewald-Born theory leads to an explanation of the change of the index of refraction with the density, and of the different photoelastic properties of NaCl, KCl, CaF_2 and diamond. The photoelastic constants of other crystals are predicted. It is shown that the "cavity" method of Lorentz and Bragg gives the same Lorentz force as the theory of Born and Ewald. The calculations of the photoelastic effect by Herzfeld and Banerjee are incorrect and incomplete.

If a cubic crystal is subjected to a pressure normal to a cube face, it becomes tetragonal, and hence doubly refracting. According to Ewald[1] and Born[2] the birefringence of crystals is due to the anisotropy of the Lorentz-Lorenz force. In ionic crystals the anisotropy of the Coulomb forces is an additional cause of birefringence. Taking into account both effects, Hylleraas[3] calculated the optical properties of calomel, rutile, anatas and quartz. For carbonates and nitrates, W. L. Bragg[4] developed a somewhat different theory in which the birefringence is primarily due to the optical anisotropy of the CO_3 or NO_3 groups.

The success of these theories gives reason to anticipate that they could also explain the accidental double refraction of cubic crystals. We shall show that, in general, this expectation is not justified. Neither Ewald-Born's nor Bragg's theory can explain the photoelastic behavior of cubic crystals, except in some special cases. This conclusion has been reached previously by Herzfeld,[5] Herzfeld and Lee, and Banerjee.[6] It will, however, be demonstrated here that Herzfeld's papers contain a numerical error and that Banerjee's method is wrong. Hence their results are not conclusive.

In a previous paper the writer[7] has shown that a third cause of the photoelastic effect must be considered. A deformation of the lattice changes the energy levels and transition probabilities of the optical electrons, and hence alters the refraction of the atoms. This effect is a generalization of the results of Fajans and Joos[8] who showed that in crystals the refraction of the ions are usually smaller than in solutions. We assume that a decrease of the lattice constant reduces the refractions still further. But, contrary to Fajans and Joos, we do not believe that this effect is due to the Coulomb forces between the ions. The effect exists also in homopolar crystals. It is caused by a change of the charge distribution or the binding of the optical electrons. It can be considered as produced by the repulsive forces between the atoms[9] and depends primarily on the arrangement of, and the distances between nearest neighboring atoms.

In photoelastic experiments the lattice distances parallel to the pressure are decreased, and the distances normal to the stress are increased. This gives rise to an anisotropy of the atomic refractions.

By taking into account all three effects we are able to give a satisfactory explanation of the observed photoelasticity of simple cubic lattices.

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[1] P. Ewald, Thesis, Munich, 1912; Ann. d. Physik **49**, 1, 117 (1916).

[2] M. Born, *Handbuch der Physik* Vol. 24, p. 770.

[3] E. Hylleraas, Zeits. f. Physik **36**, 859 (1926); Zeits. f. Krist. **65**, 469 (1927).

[4] W. L. Bragg, Proc. Roy. Soc. **A105**, 307 (1924); **A106**, 346 (1924).

[5] K. F. Herzfeld, J. Opt. Soc. Am. **17**, 26 (1928); Herzfeld and Lee, Phys. Rev. **44**, 625 (1933).

[6] K. Banerjee, Ind. J. Phys. **2**, 195 (1927).

[7] H. Mueller, Physics **6**, 179 (1935).

[8] Fajans and Joos, Zeits. f. Physik **23**, 1 (1924).

[9] The possibility that the repulsive forces may deform and even polarize an atom, giving rise to negative polarizabilities, was discussed by Heckmann, Zeits. f. Krist. **61**, 250 (1925).

Classical Theory of Photoelasticity

The phenomenological theory of photoelasticity of crystals was developed by F. Pockels.[10] The theory assumes that the elastic deformations, and not the stresses, are primarily responsible for the birefringence. The behavior of cubic crystals is characterized by three elasto-optical constants p_{11}, p_{12}, p_{44}, which for the purpose of our calculation are best defined as follows:

A simple strain z_z in the direction [001] produces uniaxial birefringence and we have

$$\begin{aligned} n-n_z&=\tfrac{1}{2}n^3p_{11}z_z,\\ n-n_x&=\tfrac{1}{2}n^3p_{12}z_z, \qquad (1)\\ n_x-n_z&=\tfrac{1}{2}n^3(p_{11}-p_{12})z_z; \end{aligned}$$

n is the index of refraction of the undeformed crystal, and n_z and n_x are the indices for light whose electric vector oscillates in the direction parallel and perpendicular to the strain.

The combination of a strain x_x' in the direction [110] and a strain $y_y'=-x_x'$ in the direction [$1\bar{1}0$] represents a shear $x_y=2x_x'$ and produces biaxial birefringence with the axis of the index ellipsoid in the directions $x'=[110]$, $y'=[1\bar{1}0]$, $z'=[001]$. Then

$$n_{x'}=n+\Delta n,\quad n_{y'}=n-\Delta n,\quad n_z=n,\quad \text{and}\quad \Delta n=-n^3p_{44}x_x'. \qquad (2)$$

The "Cauchy relation" $p_{44}=\frac{1}{2}(p_{11}-p_{12})$ holds only for amorphous solids. For hydrostatic pressure, for which $x_x=y_y=z_z=dV/3V=-d\rho/3\rho$, where ρ is the density, the index of refraction changes by

$$\begin{aligned} dn&=-\tfrac{1}{2}n^3[p_{11}z_z+p_{12}(x_x+y_y)]\\ &=(p_{11}+2p_{12})n^3d\rho/6\rho. \qquad (3) \end{aligned}$$

If $p_{11}-p_{12}>0$ a pressure normal to a cube face produces positive birefringence. This is the case[11] for KCl, KBr, KI and NH_4I. $p_{11}-p_{12}$ is negative for NaCl, CaF_2, NaF, ZnS, diamond, Al- and NH_4-alum. If p_{44} is negative, the crystal shows negative uniaxial birefringence for pressure normal to an octahedral face. This is the case for NaCl, KCl and the alums; but, for CaF_2, p_{44} is positive. A satisfactory theory must be able to account for these reversals of sign.

The comparison between theory and observation is simplified by introducing

$$\begin{aligned} p_x&=n^4p_{12}(n^2-1)^{-2}=-2n(n^2-1)^{-2}dn_x/dz_z,\\ p_z&=n^4p_{11}(n^2-1)^{-2}=-2n(n^2-1)^{-2}dn_z/dz_z,\\ p'=p_{x'}&=2n^4p_{44}(n^2-1)^{-2} \qquad (4)\\ &=-2n(n^2-1)^{-2}dn_{x'}/dx_x',\\ p=p_z-p_x&=n^4(p_{11}-p_{12})(n^2-1)^{-2}. \end{aligned}$$

The Ewald-Born Theory of the Lorentz-Lorenz Force

We consider a lattice with only one atom at the corners of the elementary cells. Each atom carries a charge $e=1$, and a continuous charge distribution of constant density $\rho=-1/\Delta$ compensates for the discrete charges. Δ is the volume of the elementary cell, which is determined by the three vectors a_1, a_2, a_3. The position of the atoms is given by the vectors $r^l=l_1a_1+l_2a_2+l_3a_3$. Except at the points r^l the electric potential ψ satisfies everywhere Poisson's equation

$$\Delta\psi=4\pi/\Delta \qquad (5)$$

and has the value[2]

$$\psi=\psi_1+\psi_2,$$

where

$$\begin{aligned} \psi_1&=\frac{4\pi}{\Delta}\sum{}' \exp\left[-\frac{1}{4\epsilon^2}|q^l|^2+j(q^lr)\right]\Big/|q^l|^2,\\ \psi_2&=\sum G(\epsilon|r^l-r|)/|r^l-r|-\pi/\epsilon^2\Delta; \end{aligned} \qquad (6)$$

$j=\sqrt{(-1)}$, ϵ is an arbitrary parameter; $q^l=2\pi(l_1b_1+l_2b_2+l_3b_3)$, where $b_1=[a_2\times a_3]/\Delta$, etc., are the vectors of the reciprocal lattice; $G(x)=1-2\pi^{-\frac{1}{2}}\int_0^x e^{-\alpha^2}d\alpha$; and the summations are to be taken over all combinations (l_1, l_2, l_3), excepting (0, 0, 0) in the summations Σ'.

Let us now consider a second lattice, geometrically identical with the first, but each lattice point carrying a charge $e=-1$ and displaced by a vector dr with respect to the atoms

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[10] F. Pockels, Wied. Ann. **37**, 151 (1889); *Lehrbuch der Kristallphysik*, Leipzig and Berlin, 1906.

[11] Johnson, *Neues Jahrbuch für Mineralogie*, 1902, Vol. II, p. 146.

of the first lattice. At the point r the second lattice produces a potential $\psi^* = -\psi + (dr \operatorname{grad} \psi)$. Since the continuous charges cancel each other, the two lattices together represent a lattice of dipoles with the moments $\mu = -dr$. Their potential is $\phi = \psi + \psi^* = -(\mu \operatorname{grad} \psi)$. In order to find the field due to all other dipoles acting on the dipole at the origin, one subtracts the field of this dipole and gets the potential $\bar{\phi} = -(\mu \cdot \operatorname{grad} \bar{\psi})$, $\bar{\psi} = \psi - 1/r$. We consider now the simple case, where all dipoles are parallel to the applied field E_x. The total field acting on any dipole is the Lorentz-Lorenz force

$$F_x = E_x - (d\bar{\phi}/dx)_0 = E_x + \mu_x(\partial^2\bar{\psi}/\partial x^2)_0$$
$$= E_x + 4\pi L_x P_x, \quad (7)$$

where $P_x = \mu_x/\Delta$ is the polarization, and where we have introduced the "Lorentz factor"

$$L_x = (\Delta/4\pi)(\partial^2\bar{\psi}/\partial x^2)_0. \quad (8)$$

From (5) it follows that $L_x + L_y + L_z = 1$, and hence for a simple cubic lattice[12] $L_x = L_y = L_z = 1/3$.

For a simple tetragonal lattice, where $a_1 = a_2 \neq a_3$, we have $L_x = L_y$, $L_z = 1 - 2L_x$. The numerical calculation is conveniently carried out for $L_x - L_z$. Choosing $\epsilon = \pi^{-\frac{1}{2}}\Delta^{-\frac{1}{3}}$ we get

$$L_x - L_z = -\sum{}'(Q_x - Q_z)Q^{-1} \exp(-Q)$$
$$+ \sum{}'(R_x - R_z)(3/2R + 1)R^{-1} \exp(-R)$$
$$+ (3\pi^{\frac{1}{2}}/4)\sum(R_x - R_z)R^{-5/2}G(R^{\frac{1}{2}}), \quad (9)$$

where

$$Q = Q_x + Q_y + Q_z = \pi\Delta^{\frac{2}{3}}(l_1^2/a_1^2 + l_2^2/a_2^2 + l_3^2/a_3^2),$$
$$R = R_x + R_y + R_z = \pi\Delta^{-\frac{2}{3}}(l_1^2 a_1^2 + l_2^2 a_2^2 + l_3^2 a_3^2).$$

All the series in (9) converge very rapidly. The values of L_x and L_z depend only on the ratio a_3/a_1.

The results in Fig. 1 show that for $a_3/a_1 > 2$ they can be represented by the approximation $L_z = 1 - 2L_x = 1 - 0.72\ a_3/a_1$. For $a_3/a_1 > 1.4$ and for $a_3/a_1 < 0.6$ one Lorentz factor becomes negative. Hence in many crystals the interaction between the dipoles does not increase, but decreases the polarization.[13]

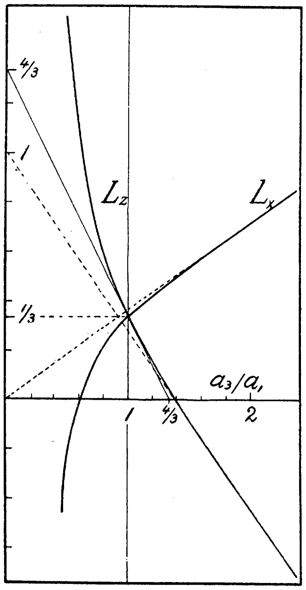

FIG. 1. The Lorentz factor for simple tetragonal lattices.

If $a_3/a_1 < 1$ the crystal is a chain lattice. For light oscillating parallel to the chains the L factor is larger than for light oscillating normal to the chains. Hence chain lattices show positive birefringence. On the other hand, for layer lattices, where $a_3/a_1 > 1$, the L factor is small for light oscillating normal to the layers and the birefringence is negative. The observations verify these rules for arbitrary layer and chain lattices.[14]

In the problem of photoelasticity of cubic crystals we are interested in the values of L_x and L_z for a lattice which differs only slightly from a cubic lattice. A strain z_z produces an axial ratio $a_1 : a_2 : a_3 = 1 : 1 : (1 + z_z)$ and the L factors differ from $\frac{1}{3}$ by small amounts; hence

$$L_x = L_y = \tfrac{1}{3} + s_x z_z; \quad L_z = \tfrac{1}{3} + s_z z_z \quad (10)$$

and we must have $2s_x + s_z = 0$. (11)

The differentiation $s_x = dL_x/dz_z$ leads to com-

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[12] The same derivation of the factor $\frac{1}{3}$ can also be used for a random distribution of atoms. Another derivation by Darwin, Proc. Roy. Soc. **A146**, 17 (1934).

[13] In these cases Havelock's assumption (Proc. Roy. Soc. **A80**, 31 (1908)), which replaces Lorentz's spherical cavity by an ellipsoid, cannot hold. Negative Lorentz factors can be used to explain the fact that the anomalous dielectric properties of Rochelle salt occur only for fields in direction of the a axis (H. Mueller, Phys. Rev. **47**, 175 (1935)).

[14] W. A. Wooster, Zeits. f. Krist. **80**, 495 (1931).

plicated expressions. Much less numerical work is involved in calculating the difference quotient $s_x = \{L_x(1+z_z) - \frac{1}{3}\}/z_z$. By choosing $z_z = 0.01$ we obtain sufficiently accurate values. Thus we get for simple cubic lattices $L_x(1.01) = 0.33832$, $L_z(1.01) = 0.32333$, and hence $s_x = 0.499$, $s_z = -1.000$. These values agree with Herzfeld's results $s_x = 0.501$, $s_z = -1.01$, which are calculated from Madelung's lattice potential. From Banerjee's calculation we derive $s_x = 0.5045$, $s_z = -1.0090$.

The Lorentz-Lorenz Force in Strained *D* Lattices*

If the elementary cells contain several different atoms at the positions r_i, r_k, etc., carrying the moments μ_{kx}, one must find the field of all other dipoles acting on an atom i. This leads to the Lorentz factors L_{ikx} and the Lorentz force[15]

$$F_{ix} = E_x + 4\pi \sum_k L_{ikx} P_{kx}; \quad P_{kx} = \mu_{kx}/\Delta. \tag{12}$$

If the elementary cell is orthorhombic, one finds by choosing again $\epsilon = \pi^{-\frac{1}{2}}\Delta^{-\frac{1}{3}}$

$$\begin{aligned} L_{iix} &= (\Delta/4\pi)(\partial^2\bar{\psi}/\partial x^2)_0 \\ &= \tfrac{1}{3} - \textstyle\sum' Q_x Q^{-1} \exp(-Q) \\ &\quad + \textstyle\sum' R_x R^{-1} \exp(-R) \\ &\quad + \tfrac{1}{2}\textstyle\sum' (3R_x R^{-1} - 1) R^{-1} \exp(-R) \\ &\quad + (\pi^{\frac{1}{2}}/4)\textstyle\sum' (3R_x R^{-1} - 1) R^{-\frac{3}{2}} G(R^{+\frac{1}{2}}), \end{aligned} \tag{13}$$

$$\begin{aligned} L_{ikx} &= (\Delta/4\pi)(\partial^2\psi/\partial x^2)_{r_{ik}} \\ &= -\textstyle\sum' Q_x Q^{-1} \exp[-Q + j(q^l r_{ik})] \\ &\quad + \textstyle\sum R_{ikx} R_{ik}^{-1} \exp(-R_{ik}) \\ &\quad + \tfrac{1}{2}\textstyle\sum (3R_{ikx} R_{ik}^{-1} - 1) R_{ik}^{-1} \exp(-R_{ik}) \\ &\quad + (\pi^{\frac{1}{2}}/4)\textstyle\sum (3R_{ikx} R_{ik}^{-1} - 1) R_{ik}^{-\frac{3}{2}} G(R_{ik}^{+\frac{1}{2}}), \end{aligned} \tag{14}$$

and analogous equations for L_{iky} and L_{ikz}. Q and R are defined by (10) and $R_{ik} = R_{ikx} + R_{iky} + R_{ikz} = \pi\Delta^{-\frac{2}{3}}[(l_1a_1 - x_{ik})^2 + (l_2a_2 - y_{ik})^2 + (l_3a_3 - z_{ik})^2]$ where x_{ik}, y_{ik}, z_{ik} are the components of the vector $r_{ik} = r_i - r_k$. From (5) it follows that for all indices ik

$$L_{ikx} + L_{iky} + L_{ikz} = 1. \tag{15}$$

These equations serve to calculate the Lorentz factors for elastically deformed diagonal lattices. For undeformed D lattices (15) leads to $\Sigma L_{ikx} P_{kx} = \frac{1}{3} P_x$, and the Lorentz-Lorenz equation is valid. To determine the L factors for any D lattice which is deformed by a strain $z_z = 0.01$ or a shear $x_y/2 = x_x' = -y_y' = 0.01$, it is only necessary to carry out the calculations for the three orthorhombic cells shown in Fig. 2. The symmetry of these cells requires that for fields parallel to the edges of the cells all dipole moments be parallel to the electric field. Hence $L_{ikxy} = 0$, excepting $L_{ikxx} = L_{ikx}$. For reasons of symmetry $L_{ikx} = L_{kix}$ and there are a large number of relations between the 48 L factors given below.[16]

Since for an undeformed D lattice $F = E + 4\pi P/3$, we write for a lattice deformed by a strain z_z

$$F_{ix} = E_x + (4\pi/\Delta)\textstyle\sum n_k \mu_{kx} (\tfrac{1}{3} + s_{ikx} z_z). \tag{16}$$

For a shear $x_x' = -y_y' = x_y/2$ we write

$$F_{ix'} = E_x + (4\pi/\Delta)\textstyle\sum n_k \mu_{kx'} (\tfrac{1}{3} + s_{ikx'} x_x'). \tag{17}$$

Table I. *Lorentz factors*. In cell A we have $a_1 : a_2 : a_3 = 1 : 1 : 1.01$, in cell B $a_1 : a_2 : a_3 = 1.01 : 0.99 : 2^{\frac{1}{2}}$, and in cell C $a_1 : a_2 : a_3 = 1.01 : 0.99 : 2^{-\frac{1}{2}}$.

Cell A				Cell B			
ik	L_{ikx}	L_{iky}	L_{ikz}	ik	L_{ikx}	L_{iky}	L_{ikz}
11	0.3383	0.3383	0.3233	11	0.4858	0.5258	−0.0116
12	2.7528	−.8710	−.8818	12	.1689	.1530	.6781
13	−.8710	2.7528	−.8818	13	−.2716	−.2584	1.5300
14	−.8340	−.8384	2.6768	14	.9637	.8996	−.8633
15	$.3286_5$	$.3286_5$	−.3427			Cell C	
16	−.3509	.6634	.6875	11	0.1077	0.1337	0.7586
17	.6634	−.3509	.6875	12	.5664	.5262	−.0926
18	$.6837_5$	$.6837_5$	−.3675	13	−.5359	1.1866	.3494
				14	1.1706	−.4882	.3176

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* In Born's diagonal or D lattices the atoms of the elementary cell are located on the body diagonal of the elementary cube. The face- and body-centered cubic lattice, and the lattices of diamond, NaCl, CsCl, CaF_2 and ZnS are D lattices.

[15] In the general case, the dipole moments μ_k are not all parallel to the applied field and the Lorentz force is $F_{ix} = E_x + 4\pi\Sigma_k\Sigma_y L_{ikxy} P_{ky}$. We consider here only such cases where the symmetry of the crystal requires that $L_{ikxy} = 0$ for $x \neq y$.

[16] There are 16 relations due to Eq. (15). For cell A there exist 10 obvious equalities $L_{ikx} = L_{iky}$, 3 relations $\Sigma_k L_{1kx} = 8L_{11x}$, and 4 relations with the results in Fig. 1, as, for instance $\frac{1}{4}(L_{11x} + L_{12x} + L_{13x} + L_{14x}) = L_x(2.02)$. Similar relations exist for cell B and C, and there are 8 relations connecting the results for different cells. In the calculation we have not made use of any of these relations. The fact that all are satisfied shows that the errors cannot be larger than 0.0001. In the summations terms smaller than 0.00002 were neglected. All series converge very rapidly. We find the "Lorentz factors" given in Table I.

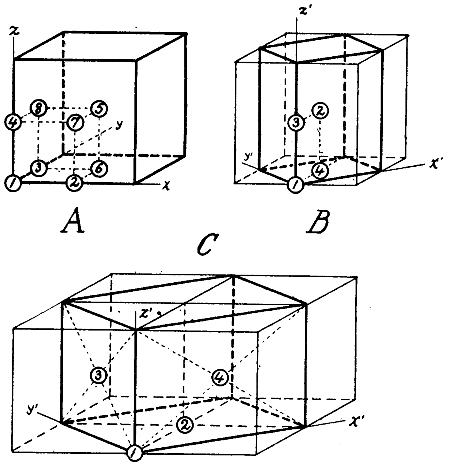

FIG. 2. Orthorhombic cells.

TABLE II. *Change of Lorentz-factor with deformation.*

CRYSTAL TYPE	*SC*	*FC*	*BC*	NaCl	CsCl	ZnS	CaF₂		DI
$s_{11x}=s_{11y}$	0.50	0.03	0.01_5	0.03	0.50	0.03	0.03	0.50	−0.22
s_{11z}	−1.00	−.06	−.03	−.06	−1.00	−.06	−.06	−1.00	.44
$s_{12x}=s_{21y}$				.97	−.47	−.47	−.47	−.47	
s_{12z}				−1.94	.94	.94	.94	.94	
$s_{11x'}=-s_{11y'}$	.33	−.60	−.62	−.60	.33	−.60	−.60	.33	−1.09
$s_{12x'}$				1.26	−1.58	−1.58	−1.58	−1.58	

n_k is the number of atoms of the kind k within an elementary cell. Replacing again the derivative by the difference quotient, we can now calculate the factors s_{ikx}, s_{ikz}, $s_{ikx'}$, etc. The cell A gives the factors s_{ikx} for the simple cubic (SC), body centered (BC), and face centered (FC) cubic lattices, and for the lattice types of NaCl, CsCl, ZnS, CaF$_2$ and diamond (DI). The cell B furnishes the factors $s_{ikx'}$ for (SC), (FC) and NaCl, and cell C gives these factors for (BC), CsCl, ZnS, CaF$_2$ and DI. For instance we get for the NaCl lattice

$$s_{11x}=s_{11y}=100\{\tfrac{1}{4}(L_{11x}+L_{16x}+L_{17x}+L_{18x})_A-\tfrac{1}{3}\},$$

$$s_{12x}=s_{21x}=100\{\tfrac{1}{4}(L_{12x}+L_{13x}+L_{14x}+L_{15x})_A-\tfrac{1}{3}\},$$

$$s_{11x'}=s_{22x'}=-s_{11y'}=100\{\tfrac{1}{2}(L_{11x}+L_{12x})_B-\tfrac{1}{3}\},$$

$$s_{12x'}=-s_{12y'}=s_{21x'}=100\{\tfrac{1}{2}(L_{13x}+L_{14x})_B-\tfrac{1}{3}\}.$$

Similar expressions give the s_{ikx} for the other lattice types. The symmetry of all lattices requires $s_{ikx}=s_{iky}$ and $s_{ikx'}=-s_{iky'}$ and from (15) it follows that $s_{ikz}=-2s_{ikx}$ and $s_{ikz'}=0$. For NaCl, CsCl, and ZnS we have evidently $s_{11x}=s_{22x}$, but for CaF$_2$ this is not true.[17]

The factors s_{ikx} and $s_{ikx'}$ in Table II determine the change of the Lorentz-Lorenz force produced by a uniform strain or shear. Our calculation does not,[18] however, take into account the "inner displacements" which occur for shear in ZnS and CaF$_2$.

These values agree neither with Herzfeld's nor with Banerjee's results. Comparison with Herzfeld's notation shows (his Eq. (12)) that his values α and β give for the NaCl lattice

$$\begin{aligned} s_{11z}&=0.585-\tfrac{2}{3}=-0.082\\ s_{12z}&=-1.248-\tfrac{2}{3}=-1.915\\ s_{11x}&=0.081-\tfrac{2}{3}=-0.586\\ s_{12x}&=2.255-\tfrac{2}{3}=1.588.\end{aligned}$$

s_{11z} and s_{12z} are in fair agreement with our values, but s_{11x} and s_{12x} are not. Since Poisson's equation requires $s_{11z}=-2s_{11x}$ and $s_{12z}=-2s_{12x}$, Herzfeld's values of s_{11x} and s_{12x} must be wrong.[19] Herzfeld's calculation is marred only by a numerical error, whereas Banerjee's method contains a fundamental error which is discussed in the next section.

BRAGG'S THEORY OF THE LORENTZ-LORENZ FORCE

Bragg's method is based on the classical procedure of H. A. Lorentz. One considers a spherical or cubical boundary around the chosen atom. The solid outside the boundary is considered

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[17] For CaF$_2$ the first column in Table II refers to Ca, the second to F.

[18] These displacements, which give rise to the piezoelectric effect and invalidate the Cauchy relation for the elastic constants, complicate our problem considerably. They lead to $L_{ikxy}\neq 0$. We neglect this effect, because the magnitude of the displacements is not known.

[19] The relation between s_{ik} and α, β was communicated to the writer by Professor Herzfeld. Professor Herzfeld agrees that his values, −0.081 and 2.255, are incorrect. He has asked me to call attention to the following corrections to his paper (J. Opt. Soc. Am. **17**, 26 (1928)): The first formula on p. 31 has the wrong sign and is incomplete. (The corresponding equation in the appendix is almost correct.) The factor 3 in the next formula should be omitted. In the second equation in the appendix, $(3+1)$ should be replaced by $(3+\frac{1}{3})$ and, in the first formula on p. 36 some coefficients are wrong. A recalculation, carried out by Dr. M. Goeppert-Mayer, gives, for stress parallel to the field, $\alpha=-0.590$ and $\beta=1.276$. Using Poisson's equation, this gives for stress normal to the field $\alpha=-.706$, $\beta=-1.638$. These new values give $s_{11x}=0.039$, $s_{12x}=0.971$, $s_{11z}=-0.077$, $s_{12z}=-1.943$. They are in good agreement with our values, which have an accuracy of ±0.01.

continuous matter, and one adds to the field of this polarized continuum the field of the dipoles within the boundary. Banerjee[6] applies this method in the following manner. He considers a cubical boundary. The field of the continuum is then $4\pi P/3$ and the field of the dipoles within the cube is $F_x' = 3\sum \mu_{ix} x_i^2/r_i^5 - \sum \mu_{ix}/r_i^3$. In the undeformed state the latter vanishes for D lattices. Deformation due to a strain z_z changes the coordinates of each dipole from x_i, y_i, z_i to x_i, y_i, $z_i(1+z_z)$ and the field of the dipoles within the boundary can be developed in powers of z_z. In first approximation

$$F_x' = z_z[3\sum \mu_{ix} z_i^2/r_i^5 - 15\sum \mu_{ix} x_i^2 z_i^2/r_i^7],$$

$$F_y' = z_z[3\sum \mu_{iy} z_i^2/r_i^5 - 15\sum \mu_{iy} y_i^2 z_i^2/r_i^7],$$

$$F_z' = z_z[9\sum \mu_{iz} z_i^2/r_i^5 - 15\sum \mu_{iz} z_i^4/r_i^7].$$

Banerjee calculates these sums for the NaCl and CaF_2 lattice. His results can be written $F_{1x}' = 8z_z\Delta^{-1}[B_{11x}\mu_{1x} + B_{12x}\mu_{2x}]$, where the B_{ikx} are the numerical values of the finite lattice sums. Since these sums contain only the coordinates of the atoms in the undeformed state, Banerjee extends the summations over a cube. But this is wrong. The atoms which are within a cube in the deformed state, are not within a cube in the original state. In other words, Banerjee does not calculate the field of the atoms contained in a cube of the deformed crystal, but of the atoms within a rectangular box with the dimensions $A_x : A_y : A_z = 1 : 1 : (1+z_z)$. Hence the field of the continuum is not $F'' = 4\pi P/3$ but

$$F_x'' = 4P_x \sin^{-1}\{2A_xA_yA_z(A_x^2+A_y^2+A_z^2)^{\frac{1}{2}}/(A_x^2+A_y^2)\cdot(A_x^2+A_z^2)\}.$$

This gives, in first approximation

$$F_x'' = 4\pi P_x/3 + 4P_x 3^{-\frac{1}{2}} z_z,$$
$$F_z'' = 4\pi P_z/3 - 8P_z 3^{-\frac{1}{2}} z_z$$

and the Lorentz-Lorenz forces are therefore

$$\begin{aligned} F_{ix} &= E_x + F_{ix}' + F_x'' \\ &= E_x + 4\pi\Delta^{-1}\sum n_k\mu_{kx} \\ &\qquad \times[\tfrac{1}{3} + z_z(2B_{ikx}\pi^{-1}n_k^{-1} + \pi^{-1}3^{-\frac{1}{2}})], \end{aligned}$$

$$\begin{aligned} F_{iz} &= E_z + F_{iz}' + F_z'' \\ &= E_z + 4\pi\Delta^{-1}\sum n_k\mu_{kz} \\ &\qquad \times[\tfrac{1}{3} + z_z(2B_{ikz}\pi^{-1}n_k^{-1} - 2\times 3^{-\frac{1}{2}}\pi^{-1})]. \end{aligned}$$

Comparison with (16) gives

$$s_{ikx} = 2B_{ikx}/\pi n_k + 3^{-\frac{1}{2}}\pi^{-1},$$

$$s_{ikz} = 2B_{ikz}/\pi n_k - 2\times 3^{-\frac{1}{2}}\pi^{-1}$$

and we can calculate s_{ikx} from Banerjee's value of B_{ikx}. For NaCl we get, since $n_1 = n_2 = 4$

$$s_{11z} = -2s_{11x} = 1.9005/2\pi - 2\times 3^{-\frac{1}{2}}\pi^{-1} = -0.0651,$$

$$s_{12z} = -2s_{12x} = -9.9613/2\pi - 2\times 3^{-\frac{1}{2}}\pi^{-1} = -1.9529.$$

For CaF_2, where $n_1 = 4$, $n_2 = 8$,

$$s_{11z} = -0.0651,$$

$$s_{22z} = -2s_{22x} = -8.0608/4\pi - 2\times 3^{-\frac{1}{2}}\pi^{-1} = -1.0090,$$

$$s_{12z} = -2s_{12x} = 16.4904/4\pi - 2\times 3^{-\frac{1}{2}}\pi^{-1} = 0.9447.$$

In Banerjee's paper the terms $2\times 3^{-\frac{1}{2}}\pi^{-1}$ are neglected.[20]

The agreement between these and our previous results shows that the Ewald-Born and the Lorentz-Bragg methods are equivalent.

THE ANISOTROPY OF THE COULOMB FORCES

In an ionic lattice the potential of an atom i due to the charges $z_k\epsilon$ of all the other ions is $V_i = z_i\epsilon\psi(0) + \epsilon\sum' z_k\psi(r_{ik})$ ϵ is the positive value of the electronic charge and z_k is the valence of the ions k. The equilibrium condition demands $(\text{grad } V_i)_0 = 0$.

Under the influence of a light wave oscillating in the x direction the atom i becomes an oscillator. With Born[2] we make the assumption that the oscillator can be considered as a vibrating "electron" with the charge $-f_i\epsilon$. The forces acting on this electron are the binding force of the atom i, the Lorentz force of the light wave, and the Coulomb forces of all other ions. If the electron has a displacement u_{ix} from its rest position, the Coulomb field is

$$F_{ix}^c = -(\partial^2 V_i/\partial x^2)_0 \cdot u_{ix} = -\epsilon u_{ix}[z_i(\partial^2\bar{\psi}/\partial x^2)_0 + \sum_{i\neq k} z_k(\partial^2\psi/\partial x^2)_{r_{ik}}].$$

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[20] It is surprising that, in spite of this large error, Banerjee finds reasonable results. This is probably due to his questionable method for calculating the refractive index (Banerjee's Eq. (6) and (8)). We have not succeeded in correcting his calculations for shear.

In a D lattice it follows from (15) that $(\partial^2\bar{\psi}/\partial x^2)_0 = (\partial^2\psi/\partial x^2)_{r_{ik}} = 4\pi/3\Delta$ and hence $F_{ix}{}^c = -\epsilon u_{ix}4\pi/3\Delta\cdot\sum z_k = 0$ because of the neutrality condition. Hence the Coulomb forces do not influence the refraction of D lattices.

In an elastically deformed D lattice, we get, using (13) and (14) $F_{ix}{}^c = -4\pi\epsilon u_{ix}\Delta^{-1}\sum z_k L_{ikx}$. Since $-u_{ix}f_i\epsilon = \mu_{ix}$, $\sum z_k = 0$, this can also be written

$$F_{ix}{}^c = 4\pi\mu_{ix}z_z(f_i\Delta)^{-1}\sum z_k n_k s_{ikx}. \tag{18}$$

Analogous equations hold for $F^c{}_{iz}$, $F^c{}_{ix'} = -F^c{}_{iy'}$. In amorphous[7] solids all $s_{ikx} = 1/15$, $s_{ikz} = -2/15$ and hence, since $\sum n_k z_k = 0$, Coulomb forces have no influence.

INFLUENCE OF HYDROSTATIC PRESSURE

Hydrostatic pressure does not change the symmetry of cubic crystals. Since $x_x = y_y = z_z$ it follows from (15) that the Lorentz factor is 1/3 and the Coulomb forces have no influence. This supports our previous statement that, in cubic crystals, the change of refraction is not due to the Coulomb forces, but is caused by a change in the binding force of the optical electrons.

The Lorentz-Lorenz equation must therefore be valid for hydrostatic pressure and should determine the change of the index of refraction n with the density ρ. Pockels[10] has calculated $dn/d\rho$ from photoelastic data, using (3), and has shown that for NaCl, CaF$_2$, and probably also for KCl, it has practically the same value as $-1/\alpha\cdot dn/dt$, where α is the coefficient of temperature expansion. But the observed increase of n with density is considerably smaller than the value given by the Lorentz-Lorenz equation. This equation can only be reconciled with the observations if we assume that a compression reduces the polarizabilities of the atoms. We must assume that a change of volume ΔV increases all refractions $R_i' = R_i(1+\lambda_i\Delta V)$ and get then

$$\begin{gathered}\rho\cdot dn/d\rho = (n^2-1)(n^2+2)(1-\lambda_0)/6n\\ \lambda_0 = \sum\lambda_i n_i R_i/\sum n_i R_i.\end{gathered} \tag{19}$$

The data in Table III show that λ_0 has, within the accuracy of the data, the same value for NaCl, KCl, and CaF$_2$, and differs but little from the value[7] 0.4 found for glasses.

TABLE III.

CRYSTAL	$\rho dn/d\rho$	$-(1/\alpha)dn/dt$	$(n^2-1)(n^2+2)/6n$	λ_0
NaCl	0.304	0.305	0.656	0.536
KCl		.30	.576	.48
CaF$_2$	.251	.22	.498	.50

OPTICAL ANISOTROPY OF THE ATOMS

It is natural to assume that in unstrained D lattices all atoms are optically isotopic. Since a hydrostatic pressure alters the refractions, a strain will produce optical anisotropy of the atoms. A distortion of the lattice produces a deformation of the atoms. We must assume a linear change of the molar refractions R_k, or the polarizabilities α_k, with the strain. If A is Avogadro's number, we have

$$\begin{gathered}R_{kx} = 4\pi A\alpha_{kx}/3 = R_{ky} = R_k(1+\lambda_{kx}z_z),\\ R_{kz} = 4\pi A\alpha_{kz}/3 = R_k(1+\lambda_{kz}z_z).\end{gathered} \tag{20}$$

For a shear we must assume

$$R_{kx'} = R_k(1+\lambda_{kx'}x_x'), \quad R_{ky'} = R_k(1+\lambda_{ky'}x_x').$$

The change of the refraction due to hydrostatic pressure is determined by $\lambda_i = \frac{1}{3}(\lambda_{iz}+2\lambda_{ix})$.

CALCULATION OF THE PHOTOELASTIC CONSTANTS

Under the influence of the Lorentz and Coulomb forces the atoms i acquire the dipole moments $\mu_{ix} = \alpha_{ix}(F_{ix}+F_{ix}{}^c)$, where α_{ix} is the polarizability for the frequency of the lightwave. Introducing the expressions from Eqs. (16), (18) and (20), we get a set of linear equations for the moments μ_{ix}

$$\mu_{ix} = 3R_i(1+\lambda_{ix}z_z)A^{-1}[E_x/4\pi + \Delta^{-1}\sum n_k\mu_{kx}(\tfrac{1}{3}+s_{ikx}z_z) + \mu_{ix}z_z(f_i\Delta)^{-1}\sum z_k n_k s_{ikx}].$$

From their solutions we determine

$$(n_x{}^2-1)/4\pi = P_x/E_x = \sum n_k\mu_{kx}/E_x. \tag{21}$$

For $z_z = 0$, one finds the Lorentz-Lorenz equation $(n^2-1)/(n^2+2) = \sum n_k R_k/A\Delta$. Differentiation of (21) gives, according to (4), p_x, and in the same way one determines p_z and $p_{x'}$. In differentiating we must take into account the fact that a strain z_z changes the volume Δ of the elementary cell. The final result can be written

$$\begin{aligned} p_x &= p_0+p_x{}^L+p_x{}^c+p_x{}^A, \\ p_z &= p_0+p_z{}^L+p_z{}^c+p_z{}^A, \\ p_{x'} &= \qquad p^L{}_{x'}+p^c{}_{x'}+p^A{}_{x'}. \end{aligned} \tag{22}$$

p_0 is due to the change of the density

$$p_0=(n^2+2)/3(n^2-1). \tag{23}$$

This term is responsible for the fact that p_{11} and p_{12} always have positive values. $p_x{}^L$ is due to the anisotropy of the Lorentz force

$$p_x{}^L=-\sum_{i,\,k} s_{ikx}n_in_kR_iR_k/(\sum n_kR_k)^2, \tag{24}$$

$p_x{}^c$ gives the effect produced by the Coulomb field of the ions

$$p_x{}^c=-\sum R_i{}^2n_if_i{}^{-1}\sum_k n_kz_ks_{ikx}/(\sum n_kR_k)^2. \tag{25}$$

If the refraction of the atoms i is represented by a set of oscillators with the refractions R_{it} and strengths f_{it}, one must substitute $R_i{}^2/f_i=\sum R_{it}{}^2/f_{it}$; $R_i=\sum R_{it}$. $p_x{}^A$ is the contribution of the optical anisotropy of the atoms due to strains

$$p_x{}^A=-(n^2+2)\lambda_x/3(n^2-1), \tag{26}$$

where

$$\lambda_x=\sum\lambda_{ix}n_iR_i/\sum n_iR_i.$$

Equations analogous to (24), (25), (26) give $p_z{}^L$, $p^L{}_{x'}$, etc. Finally we write

$$p=p_z-p_x=p^L+p^c+p^A, \tag{27}$$

where, since for all D lattices $s_{ikz}=-2s_{ikx}$, $p^L=-3p_x{}^L$, $p^c=-3p_x{}^c$, $p^A=-\lambda(n^2+2)/3(n^2-1)$; $\lambda=\lambda_z-\lambda_x$. λ_0, which determines the change of refraction due to hydrostatic pressure, is

$$\lambda_0=\tfrac{1}{3}(\lambda_z+2\lambda_x). \tag{28}$$

The shear constant of photoelasticity is given by

$$p'=p'^L+p'^c+p'^A, \tag{29}$$

where

$$p'^L=p^L{}_{x'};\ p'^c=p^c{}_{x'};\ p'^A=-\lambda'(n^2+2)/3(n^2-1);$$
$$\lambda'=\sum\tfrac{1}{2}(\lambda_{ix'}-\lambda_{iy'})n_iR_i/\sum n_iR_i.$$

Eqs. (27) and (29) represent our final result. They give p and p', which, according to (4), are proportional to the elasto-optical constants.

COMPARISON WITH EXPERIMENTAL RESULTS

In the experiments the accidental birefringence is measured as a function of the applied pressure. If C is the difference in optical path of the ordinary and extraordinary ray produced by a pressure of 1 dyne/cm² directed normal to the light path of 1 cm length, then

$$p_{11}-p_{12}=2\lambda C_1/n^3(s_{11}-s_{12});$$
$$p_{44}=2\lambda C_2/n^3s_{44}.$$

Here λ is the wavelength of the light, s_{ik} are Voigt's elastic moduli, and C_1 and C_2 refer to pressure normal to the cube and octahedral faces, respectively. If the pressure is normal to a dodecahedral face, one gets[21] $C_3=C_2$, $C_4=\frac{1}{2}(C_1+C_2)$, where C_3 and C_4 are for light normal to dodecahedral and cubic faces, respectively. Only determinations of C for small pressures have a physical significance. Large pressures produce translation gliding and lead to irreversible effects.[22]

Reliable determinations of all the quantities C_i, s_{ik} and n are available only for NaCl, KCl and CaF_2.[23] They refer to sodium light and give for NaCl $p=-0.124$, $p'=-0.065$; for KCl $p=0.179$, $p'=-0.182$ and for CaF_2 $p=-0.653$, $p'=0.179$.

For crystals of the type NaCl the theory gives

$$p=(R_1+R_2)^{-2}[0.09(R_1{}^2+R_2{}^2)+5.82R_1R_2+2.82z(R_1{}^2/f_1-R_2{}^2/f_2)]-\lambda(n^2+2)/3(n^2-1), \tag{30}$$

$$p'=(R_1+R_2)^{-2}[0.60(R_1{}^2+R_2{}^2)-2.52R_1R_2-1.86z(R_1{}^2/f_1-R_2{}^2/f_2)]-\lambda'(n^2+2)/3(n^2-1). \tag{31}$$

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[21] Pockels' data verify these relations, but Banerjee's data give slightly different results. According to our theory we must expect deviations from Pockels' theory, because the λ_{ix} are not components of a simple tensor.

[22] The results of Maris, J. Opt. Soc. Am. **15**, 194 (1927) are probably due to this effect. This is shown by Ritzel, Zeits. f. Krist. **52**, 275 (1912).

[23] The values for NaCl are averages calculated from the

The index 1 refers to the negative ion, and z is the valence of both ions.

Under a pressure normal to a cube face the NaCl lattice approaches the structure of a chain lattice. Consequently the influence of the Lorentz force given by the first two terms of (30) produces positive birefringence. The next terms are due to the Coulomb forces. The negative ions give a positive contribution because they are surrounded by positive ions which attract the optical electron. A pressure increases this attraction in the direction of the stress, and hence this gives rise to positive birefringence. For the positive ions this effect is reversed, but, since in most cases $R_1 > R_2$, the net effect of the Coulomb forces is a positive double refraction. Hence in every case the Born-Ewald theory gives positive birefringence for any NaCl lattice compressed normal to a cube face. The fact that sodium chloride shows negative birefringence shows clearly the importance of the optical anisotropy of the atoms due to pressure. We conclude that p is the difference between two large terms of equal magnitude, and this explains why it is always small for NaCl lattices, and why it can be positive or negative.

For pressure normal to an octahedral face the Lorentz force gives either a small positive or a negative effect. But the Coulomb forces and the anisotropy produce negative birefringence, and hence p' is always negative for NaCl lattices.

A quantitative test of the theory requires the values of R and f. The ionic refractions are known with a satisfactory degree of accuracy. However, very little is known concerning the strengths f_i of the oscillators. Herzfeld and Wolf[24] have shown that for ions f probably has the same values as for the corresponding inert gases. We shall base our calculation on this assumption, but we are aware that this may be incorrect. From the point of view of the quantum theory of dispersion there is even some doubt whether our f values are identical with the strength of the oscillators.[25]

If we use for NaCl and KCl the values given by Herzfeld and Wolf, we get

for NaCl $p = 0.401 + 0.597 - 1.055\lambda$; $p' = 0.392 - 0.394 - 1.055\lambda'$;

for KCl $p = 1.008 + 0.426 - 1.152\lambda$; $p' = 0.005 - 0.282 - 1.152\lambda'$.

To get agreement with the experimental results, we must have for NaCl, $\lambda = 1.06$, $\lambda' = 0.06$; for KCl, $\lambda = 1.08$, $\lambda' = -0.09$.

These results are very satisfactory for the following three reasons:

(1) The order of magnitude of the values of λ is the same as for glasses. For glasses[7] we calculated $L^* \sim 0.6$, and this represents an average value between λ and λ'. From (28) and the data in Table II we get for NaCl, $\lambda_z = 1.24$, $\lambda_x = 0.18$; for KCl, $\lambda_z = 1.20$, $\lambda_x = 0.11$. This leads to the same conclusions as in our first paper. A strain of 1 percent increases the refractions parallel to the strain by about 1.2 percent. Moreover, it increases slightly the refractions perpendicular to the strain.

(2) Although they have different photoelastic properties, both crystals lead to almost identical values of all factors λ. This agrees with the fact that the refraction of NaCl and KCl is largely due to the Cl ions.

(3) In both crystals the anisotropy produced by a strain z_z is much larger than the anisotropy produced by a shear. A strain alters the distance between nearest neighboring atoms. For a shear, however, the NaCl distance remains unchanged. Hence $\lambda > \lambda'$. The optical anisotropy due to a shear is caused by the change of the Cl-Cl distance. In NaCl the Cl ions are in contact with each other because the Na ions are smaller than the Cl ions. In KCl the Cl-Cl distance is larger; hence $\lambda'_{\text{NaCl}} > \lambda'_{\text{KCl}}$. A negative value of λ' is improbable and can be avoided by choosing slightly different values of R_i and f_i.

If, as in KCl, the anion and cation are almost equal in size and structure, it is reasonable to assume $\lambda' = 0$ and $f_1 = f_2$. The shear constant of photoelasticity is then determined by the Ewald-Born theory, and this offers a unique method

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data of F. Pockels, Ann. d. Physik **39**, 440 (1890), and of K. Banerjee, Ind. J. Phys. **2**, 195 (1927). Their results differ by about 8 percent. Pockels' results for KCl are corrected by using Försterling's values of the elastic constants (Zeits. f. Physik **2**, 172 (1920)). CaF_2 was measured by Pockels, Ann. d. Physik **37**, 372 (1889). Many other investigators have verified the signs and order of magnitude of the six constants.

[24] Herzfeld and Wolf, Ann. d. Physik **78**, 35 (1925).

[25] Herzfeld and Lee, Phys. Rev. **44**, 623 (1933) conclude that f is probably larger than the strength of the oscillator.

for the determination of the ratio $r = R_1/R_2$ of the ionic refractions. Namely, it follows then from (31)

$$(1+r)^2 p' = 0.60(1+r^2) - 2.52r - 1.86(r^2-1)/f.$$

Assuming $f_K = f_{Cl} = f_{Ar} = 4.58$ leads to $r = 5.12$, and since $R_K + R_{Cl} = R_{KCl} = 10.85$ we get $R_{Cl} = 9.07$, $R_K = 1.78$. R_{Cl} is in very good agreement with the value given by Born and Heisenberg.[26] R_K is somewhat smaller than the accepted value for the free ion, $R_K = 2.23$. Agreement with the values of Fajans and Joos[8] and Pauling[27] can be reached by choosing $f = 5.9$, or by assuming a 30 percent larger experimental value. The latter alternative is not excluded because Pockels and Voigt report that their KCl crystals were optically and elastically imperfect.

For CaF_2 the theory gives, if we introduce $R_F = 2.5$, $R_{Ca} = 1.35$, $f_F = 2.37$, $f_{Ca} = 4.58$, $p = 0.46 - 0.73 - 1.28\lambda$; $p' = 0.35 + 0.48 - 1.28\lambda'$. For a pressure normal to a cube face the Lorentz force again produces positive birefringence, but this is compensated by the negative contribution of the Coulomb forces. Hence CaF_2 becomes negatively birefringent. For a pressure normal to an octahedral face the Lorentz and Coulomb forces produce positive birefringence which cannot be compensated by the relatively small anisotropy due to shear. Qualitatively the theory explains the photoelastic properties of fluorite. Quantitatively, however, we find $\lambda = 0.3$, which is certainly too small, and $\lambda' = 0.5$, which is too large. By choosing $f_F = 5$, much more sensible values, $\lambda = 0.61$, $\lambda' = 0.06$, are obtained. An investigation of the dispersion of the photoelastic effect should determine the proper choice of the f values. It is doubtful whether the inner displacements would change the result.

For diamond Wertheim[28] observed a negative stress optical constant, but he does not state the direction of pressure. The fact that the photoelastic effect can be observed even in small crystals in spite of the large elastic constants of diamond, indicates that either p or p' must have an unusually large negative value. The theory confirms that $p = -0.66 - \lambda(n^2+2)/3(n^2-1)$ is negative and at least ten to twenty times larger than for NaCl. Since the index of refraction of diamond increases with temperature,[29] λ is probably also unusually large.

Photoelasticity and Crystal Structure

Pockels[10] has classified the cubic crystals in four groups according to the signs of $(p_{11} - p_{12})$ and p_{44}, or, what is equivalent, of p and p'.

Group	p	p'	*Example*
I	+	+	none
II	−	−	NaCl
III	−	+	CaF_2
IV	+	−	KCl

Observations with crossed nicols of the interference colors produced by pressure decide to which group a crystal belongs.

In general the theory is not able to predict the sign of p and p'. Negative values are assured if the Lorentz and Coulomb forces produce negative birefringence, because the anisotropy will always give a negative effect. If p^L and p^c together give a positive value, the result depends on whether or not $(p^L + p^c)$ is large enough to compensate the effect of the anisotropy of the atoms. Since the magnitude of the latter cannot be predicted, no definite answer can be given. Our results on glasses, NaCl and KCl indicate that p^A has for most substances nearly the same value. Hence we expect a positive value of p if $(p^L + p^c) > 1$. For shear the anisotropy produces a smaller effect and hence p' will be positive if $(p'^L + p'^c) > 0.3$. The choice of these limits is somewhat arbitrary, and in border cases our conclusions will not always be justified.

Using these critical values we are now able to predict certain correlations between Pockels' groups and the various cubic lattice types. For monoatomic crystals we have $p^c = 0$, $p^L = 3s_{11x}$, and $p'^L = -s_{11x'}$. From the values in Table II we conclude that simple cubic lattices belong to group IV, face- and body-centered and diamond lattices to group III or eventually to group II. Experimental verification is only possible for diamond.

For the diatomic ionic lattice types, NaCl, CsCl and ZnS, the results depend on the ratio

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[26] Born and Heisenberg, Zeits. f. Physik **23**, 388 (1924).

[27] L. Pauling, Proc. Roy. Soc. **A114**, 181 (1927).

[28] Wertheim, Pogg. Ann. **86**, 321 (1852).

[29] A. Sella, Rend. Acc. Lincei **7**, 300 (1891).

$r = R_-/R_+$, the values of f_-, f_+ and the valency z. For all three types we have

$$p^L + p^c = 3s_{11x} + 3(s_{12x} - s_{11x}) \times (1+r)^{-2} \cdot [2r + (r^2 - f_-/f_+)z/f_-],$$

$$p'^L + p'^c = -s_{11x'} + (s_{11x'} - s_{12x'}) \times (1+r)^{-2} \cdot [2r + (r^2 - f_-/f_+)z/f_-].$$

Fig. 3 shows the variation of $p^L + p^c$ and $p'^L + p'^c$ with r. The dotted curves give p^L and p'^L. We have assumed[30] $f_-/f_+ = 1$, and have used the values $z/f_- = 0.2$ and $z/f_- = 0.4$. For most crystals z/f_- will be between these limits. For lattices of the type CaF_2 we get two sets of curves, one corresponding to CaF_2, BaF_2, etc., the other to Li_2O, Na_2O, etc. The curves in Fig. 3 are calculated for $f_- = 3$ and $f_- = 6$, $f_-/f_+ = 1$.

Fig. 3 shows that, whenever $p^L + p^c$ is large, $p'^L + p'^c$ is small or negative, and *vice versa*. Consequently, none of the lattice types considered corresponds to Pockels' group I. No crystal belonging to this group has ever been found.

For the lattice type NaCl p' is always negative; hence these crystals belong either to group II or IV. They belong to group IV if $r < 10$ or if z/f_- is large. This is the case for all K-, Rb-, Cs- and NH_4-halides, and for the bivalent salts, BaO, CaO, etc. The Na- and Li-halides, however, belong to group II. According to Fig. 3 no other lattice type belongs to group IV. This fact can therefore be used for the determination or verification of crystal structures.

The CsCl structures can belong to group II or III, but, since group II requires $r > 10$, all the Cs- and NH_4-halides will have the photoelastic properties of group III. No observations on these crystals have been made. Measurements on the ammonium-halides would furnish an interesting test of the theory because the two modifications of these crystals should show different photoelastic properties.

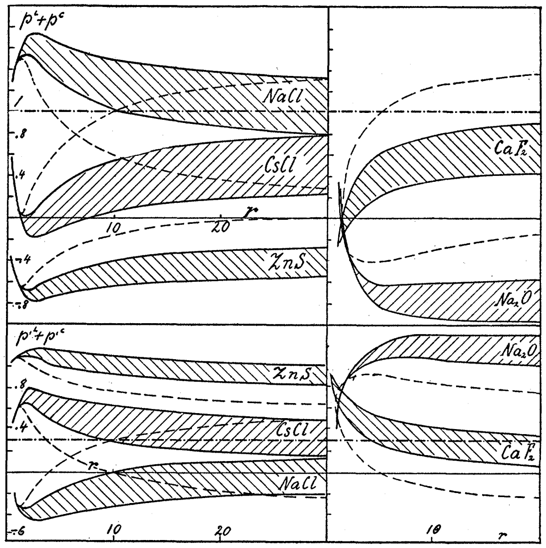

FIG. 3. Variation of photoelastic constants with ionic refraction ($r = R_-/R_+$).

Crystals of the type CaF_2 behave like CsCl and all known crystals belong to group III.

All crystals of the types ZnS and Na_2O should belong to group III irrespective of whether the binding is homopolar or ionic. For ionic crystals an unusually large effect would have to be expected.

All these conclusions agree with the known facts. The number of reliable[31] observations is very limited, and we hope to present soon further verification of the theory. An extension of the theory to more complicated lattices requires the calculation of intricate lattice sums.

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[30] In all cases where f_-/f_+ differs much from unity the ratio r is so large that the value of f_-/f_+ is immaterial.

[31] Many observers do not realize that in cubic crystals the photoelastic effect depends on the direction of pressure and observation, and their results cannot be used since they neglect to state these directions.