LATTICE-THEORY OF ALKALINE EARTH CARBONATES.

Part II. Elasticity-Constants of Aragonite.

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Introduction.

IN a preceding paper,[1] referred to hereafter as I, the lattice energy of the crystals of Aragonite and the value of n, the index of the repulsive forces were calculated. In this paper we proceed with the calculations of the elasticity-constants. In the case of such elasticity-constants, as depend on the ionic deformations, no agreement between the experimental values and the values calculated on simple theories can be expected. We restrict ourselves to the calculation of only those constants which do not essentially depend on the ionic deformation.

The method depends in being able to find out systems of parallel neutral planes in the crystal. We assume a deformation by which the distance between the consecutive planes is uniformly changed. Though the longitudinal stress in the crystal is always connected with a transversal contraction, we neglect the changes in the distances of the ions inside each plane. This amounts to assuming that the contraction has no great influence on the value of the elasticity-constants in the longitudinal direction. The results of the calculations will amply justify this procedure.

The elasticity-constant c_{jh} consists of two parts c^{e}_{jh} and c^{r}_{jh}, which are due to the electro-static and the repulsive forces, respectively. These two parts will be calculated separately.

§7. *Systems of Parallel Neutral Planes.*

Fig. 1 gives the projection of the crystal on the xy plane. Planes which are perpendicular to the x-axis are all neutral planes ; so also the planes perpendicular to the line in the x-y plane making an angle $\tan^{-1} b/3a$ with the y-axis, are all neutral. We denote this angle by θ, so that $\tan\ \theta = b/3a$ (1, 1)

[1] B. Y. Oke, *Proc. Ind. Acad. Sci.*, 1936, 4, 1.

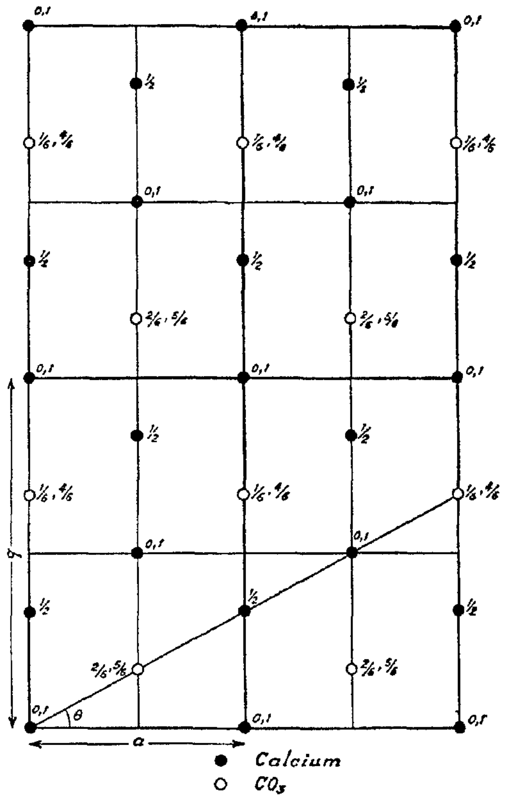

FIG. 1.

The numbers in the figure denote the ' heights ' as multiples of c above the plane $z = 0$.

In the system of parallel neutral planes perpendicular to the x-axis the distance d, between consecutive planes, is given by

$$d = a/2 \qquad \ldots \qquad (1, 2)$$

Fig. 2 shows the arrangement of the ions in the planes at $x = 0$, $\pm\, a$, $\pm\, 2a$, ... $\pm\, na$, ...

The cell of the plane-lattice consists of 4 ions whose y and z co-ordinates are given by

$$\left.\begin{array}{lll} k = 1, \text{ Calcium ion} & & (0,\ 0) \\ k = 2, \text{ Calcium} & ,, & \left(\frac{b}{3}, \frac{c}{2}\right) \\ k = 3, \ CO_3 & ,, & \left(\frac{2b}{3}, \frac{c}{6}\right) \\ k = 4, \ CO_3 & ,, & \left(\frac{2b}{3}, \frac{2c}{3}\right) \end{array}\right\} \qquad \ldots \qquad (1, 3)$$

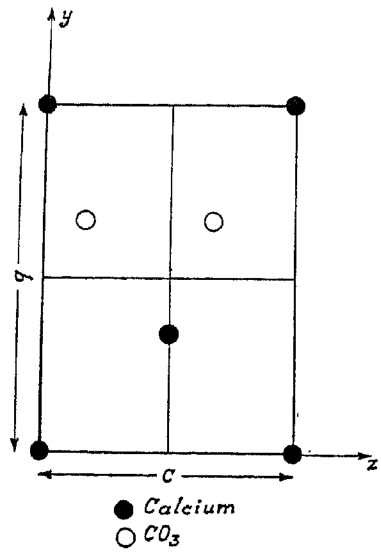

FIG. 2.

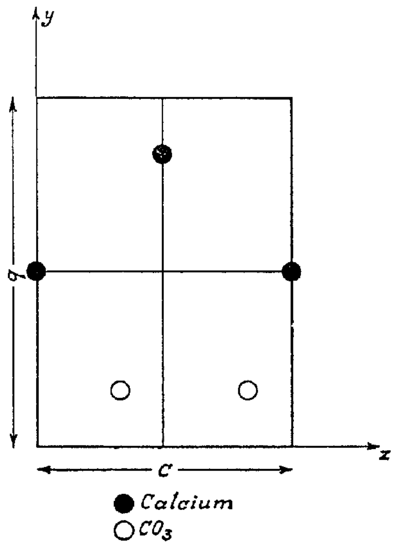

FIG. 3.

Fig. 3 shows the arrangement of the ions in the planes at

$$x = \pm \frac{a}{2}, \pm \frac{3a}{2}, \dots\dots, \pm \frac{2n+1}{2} a, \dots\dots$$

The y and z co-ordinates of the 4 ions constituting a cell of the plane-lattice are given by

$$\left.\begin{array}{llll} k = 1, & \text{Calcium ion} & & \left(\frac{b}{2}, \; 0\right) \\ k = 2, & \text{Calcium} & ,, & \left(\frac{5b}{2}, \frac{c}{2}\right) \\ k = 3, & CO_3 & ,, & \left(\frac{b}{6}, \frac{c}{3}\right) \\ k = 4, & CO_3 & ,, & \left(\frac{b}{6}, \frac{5c}{6}\right) \end{array}\right\} \quad \dots \quad \dots \quad \dots \quad (1, 4)$$

In the other system of parallel neutral planes the distance between consecutive planes is given by

$$d_\theta = \frac{ab}{\sqrt{9a^2 + b^2}} \quad \dots \quad \dots \quad \dots \quad \dots \quad \dots \quad (1, 5)$$

For the representation of this system we choose a system of co-ordinates x_θ, y_θ, z_θ such that the z_θ-axis coincides with the z-axis and Oy_θ is perpendicular to the planes. Fig. 4 shows the arrangement of the ions in the ne $y_\theta = 0$. All planes belonging to this system have exactly similar ionic arrangements ; the consecutive planes are displaced along the Ox_θ-axis through a distance a_θ given by

$$a_\theta = 3 \frac{a^2}{\sqrt{9a^2 + b^2}} \quad \cdots \quad (1, 6)$$

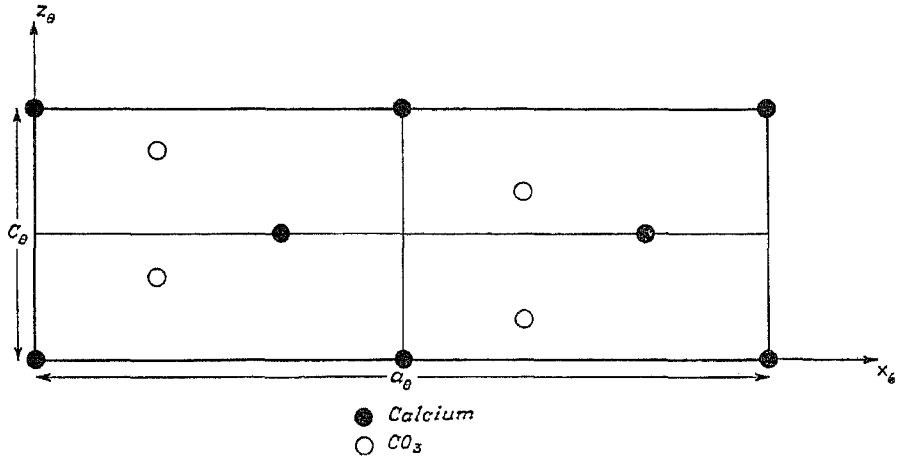

FIG. 4.

The dimensions of the unit cell of the plane-lattice are given by

$$\left.\begin{aligned} a_\theta &= \sqrt{9a^2 + b^2} \\ \text{and} \quad c_\theta &= c \end{aligned}\right\} \quad \cdots \quad (1, 7)$$

The cell consists of 8 ions, the x_θ and z_θ co-ordinates of which are given by :

$$\left.\begin{aligned} &k = 1, \text{ Calcium ion } (0, \quad 0) ; && k = 5, \text{ CO}_3 \text{ ion } \left(\frac{a_\theta}{6}, \frac{c}{3}\right) \\ &k = 2, \text{ Calcium } ,, \left(\frac{a_\theta}{3}, \frac{c}{2}\right); && k = 6, \text{ CO}_3 ,, \left(\frac{a_\theta}{6}, \frac{5c}{6}\right) \\ &k = 3, \text{ Calcium } ,, \left(\frac{a_\theta}{2}, 0\right); && k = 7, \text{ CO}_3 ,, \left(\frac{2a_\theta}{3}, \frac{c}{6}\right) \\ &k = 4, \text{ Calcium } ,, \left(\frac{5a_\theta}{6}, \frac{c}{2}\right); && k = 8, \text{ CO}_3 ,, \left(\frac{2a_\theta}{3}, \frac{2c}{3}\right) \end{aligned}\right\} \quad \cdots \quad (1, 8)$$

Denoting the elasticity constants in the directions perpendicular to the planes of these two systems by c_{11} and c_{22}^θ respectively we have

$$\left.\begin{aligned} c_{11} &= c_{11}^e + c_{11}^r \\ \text{and} \quad c_{22}^\theta &= c_{22}^{e\,\theta} + c_{22}^{r\,\theta} \end{aligned}\right\} \quad \cdots \quad (1, 9)$$

§2. *Evaluation of* c_{11}^e *and* $c_{22}^{e\,\theta}$.

We take any one of the first system of planes, say the plane $x = a/2$ and calculate the potential per unit area of this plane due to all planes on one side of this plane, say the negative side of the x-axis. Let ϕ_j (1), ϕ_j (2), ϕ_j (3) and ϕ_j (4) denote the potential at the 4 lattice points of a unit cell of the plane $x = a/2$ due to the jth adjoining plane. The potential per unit area of the plane $x = a/2$ due to the jth adjoining plane is given by

$$\Phi_j = \frac{\phi_j(1) + \phi_j(2) + \phi_j(3) + \phi_j(4)}{bc} \quad \ldots \quad \ldots \quad \ldots \quad (2,\ 1)$$

Φ, the potential per unit area due to all planes, on one side, is

$$\Phi = \sum_{j=1}^{\infty} \Phi_j \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad (2,\ 2)$$

The electro-static part of the elasticity-constant is given by

$$c_{11}^e = \frac{a}{2bc}\left[\frac{\partial^2 \Phi_1}{\partial x^2}\right]_{x=\frac{a}{2}} + \frac{a}{bc}\left[\frac{\partial^2 \Phi_2}{\partial x^2}\right]_{x=a} + \frac{3a}{2bc}\left[\frac{\partial^2 \Phi_3}{\partial x^2}\right]_{x=\frac{3a}{2}} + \cdots \ldots \quad (2,\ 3)$$

We have[2]

$$\phi_1\ (x, y, z) = \frac{2\pi}{bc}\ 2e \sum_{l,\,m}{}' \ e_{x,y,z} \frac{e^{-\alpha_{l,m}|x|}}{\alpha_{l,m}}\ e^{2\pi i\,(l\,y/b + m\,z/c)} f_1\ (l, m) \quad \ldots \quad (2,\ 4)$$

$$\text{where } \alpha_{l,m} = 2\pi \left|\frac{l}{b} + \frac{m}{c}\right| \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad (2,\ 5)$$

$$\text{and} \quad f_1\ (l, m) = (\cos 0 - i \sin 0) + \left[\cos\left(\frac{2\pi l}{3} + m\pi\right) - i \sin\left(\frac{2\pi l}{3} + m\pi\right)\right]$$
$$- \left[\cos\left(\frac{4\pi l}{3} + \frac{m\pi}{3}\right) - i \sin\left(\frac{4\pi l}{3} + \frac{m\pi}{3}\right)\right]$$
$$- \left[\cos\left(\frac{4\pi l}{3} + \frac{4m\pi}{3}\right) - i \sin\left(\frac{4l\pi}{3} + \frac{4m\pi}{3}\right)\right] \quad \ldots \quad (2,\ 6)$$

$e_{x,y,z}$ is the electric charge at the point $(x,\ y,\ z)$.

Substituting the co-ordinates from (1, 4)

$$\phi_1\ (k) = \frac{2\pi}{bc}\ (2e)^2 \sum_{l,\,m}{}' \ \frac{e^{-\alpha_{l,m}|x|}}{\alpha_{l,m}}\ F_1^{l,m}\ (k) \quad \ldots \quad \ldots \quad \ldots \quad (2,\ 7)$$

The function $F_j^{l,m}$ (k) is given by

$$F_j^{l,m}\ (k) = f_j\ (l, m) \times g_{l,m}(k) \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad (2,\ 8)$$

[2] M. Born, *Ency. der Math. Wiss.*, 3: *Physik.*, §37, p. 722, eqn. 413.

The g's are found to be as follows :—

$$\left.\begin{aligned} g_{l,m}(1) &= \cos l\pi + i \sin l\pi \\ g_{l,m}(2) &= \cos\left(\frac{5l\pi}{3} + m\pi\right) + i \sin\left(\frac{5l\pi}{3} + m\pi\right) \\ g_{l,m}(3) &= -\cos\left(\frac{l\pi}{3} + \frac{2m\pi}{3}\right) - i \sin\left(\frac{l\pi}{3} + \frac{2m\pi}{3}\right) \\ g_{l,m}(4) &= -\cos\left(\frac{l\pi}{3} + \frac{5m\pi}{3}\right) - i \sin\left(\frac{l\pi}{3} + \frac{5m\pi}{3}\right) \end{aligned}\right\} \quad .. \quad (2,\ 9)$$

For the second adjoining plane ($x = -a/2$) the function f is given by

$$f_2(l, m) = (\cos l\pi - i \sin l\pi) + [\cos(5l\pi/3 + m\pi) - \sin(5l\pi/3 + m\pi)]$$
$$- [\cos(l\pi/3 + 2m\pi/3) - i \sin(l\pi/3 + 2m\pi/3)$$
$$- [\cos(l\pi/3 + m\pi/3) - i \sin(l\pi/3 + 5m\pi/3)] \quad .. \quad (2,\ 10)$$

From (2, 1), (2, 7), (2, 8) and (2, 9)

$$\Phi_j = \frac{2\pi}{b^2c^2} 4e^2 \sum_{l,m}{}' \frac{e^{-\alpha_{l,m}|x|}}{\alpha_{l,m}} \left(\sum_{k=1}^{4} F_j^{l,m}(k) \right) .. \quad .. \quad .. \quad (2,\ 11)$$

Substituting this in (2, 3) and using (2, 5)

$$c_{11}^e = \frac{4\pi^2}{b^2c^2} 4e^2 \sum_{j=1}^{\infty} \left\{ \frac{\alpha_{l,m}|jd|}{2\pi} e^{-\alpha_{l,m}|jd|} \sum_{k=1}^{4} \left(F_j^{l,m}(k) \right) \right\} \quad .. \quad (2,\ 12)$$

We put $F_j^{|l,m|} = \sum_{k=1}^{4} \left\{ F_j^{l,m}(k) + F_j^{-l,-m}(k) \right\}$ .. .. (2, 13)

From Table I, it is apparent that the first three adjoining planes need only be considered. Substituting the final value from the table and the values of b and c from I, Table I

$$c_{11}^e = -\cdot 762 \times 10^{12} \text{ dynes/cm.}^2 .. \quad .. \quad .. \quad .. \quad (2,\ 14)$$

The evaluation of $c_{22}^{e\theta}$ is done on exactly similar lines ; the first three adjoining planes have to be considered. The value obtained is

$$c_{22}^{e\theta} = -0\cdot 608 \times 10^{12} \text{ dynes/cm.}^2 \quad .. \quad .. \quad .. \quad (2,\ 15)$$

TABLE I.

j	l'	m'	$\frac{\alpha_{l,m}\lvert jd\rvert}{2\pi}$	$e^{-\alpha_{f,m}\lvert jd\rvert}$	$\frac{\alpha_{l,m}\lvert jd\rvert}{2\pi}\times e^{-\alpha_{l,m}\lvert jd\rvert}$	$F_j^{\lvert l,m\rvert}$	$\frac{\alpha_{l,m}\lvert jd\rvert}{2\pi}\, e^{-\alpha_{l,m}\lvert jd\rvert}\times F_j^{\lvert l,m\rvert}$	
1	1	0	0·31	0·144	·044	− 18	− 0·792	
	0	1	0·43	0·067	·029	0	0	
	2	0	0·63	0·019	·011	18		+ 0·198
	1	1	0·74	0·009	·006	− 4	− 0·024	
	1	− 1	0·74	0·009	·006	− 4	− 0·024	
	0	2	0·86	0·0045	·004	12		+ 0·048
	3	0	0·94	0·003	·003	0	0	
	2	1	1·06	0·001	·001	6		+ 0·006
	2	− 1	1·06	0·001	·001	6		+ 0·006
2	1	0	0·63	0·019	·011	18		+ 0·198
	0	1	0·86	0·0045	·004	0	0	
3	1	0	0·94	·003	·003	− 18	− 0·054	
						TOTAL	− 0·894	+ 0·456
							− 0·438	

§3. *Nature of the Repulsive Forces.*

The potentials per unit cell of the crystal, due to the repulsive forces, as calculated in I with the help of the equilibrium condition is given by $2\ \beta/\delta^n$ where, from I (3, 4)

$$\beta = \frac{\alpha\ e^2}{n}\ \delta^{n-1} \quad \ldots \quad (3, 1)$$

From I (3, 8) n was found to be 6·32 for aragonite.

Let the forces between two dis-similar ions be $\frac{b_{1,2}}{r^n}$, and between two similar radicals be $\frac{b_{11}}{r^n}$ or $\frac{b_{22}}{r^n}$. Let

$$b_{11} = b_{22} = -k b_{1,2} \quad \ldots \quad (3, 2)$$

Each CO_3 ion is surrounded by 6 calcium ions projecting on the plane $z = 0$ into a hexagon and another 6 calcium ions projecting into an outer hexagon.

Of these twelve, two are situated at each of distances r_1, r_2, r_5, r_6, and one at each of r_3, r_4, r_7 and r_8, where the distances are given by :

$$\left.\begin{aligned} r_1^2 &= \frac{a^2}{4} + \frac{b^2}{36} + \frac{c^2}{9}; & r_5^2 &= a^2 + \frac{b^2}{9} + \frac{c^2}{36} \\ r_2^2 &= \frac{a^2}{4} + \frac{b^2}{36} + \frac{c^2}{36}; & r_6^2 &= a^2 + \frac{b^2}{9} + \frac{c^2}{9} \\ r_3^2 &= \frac{b^2}{9} + \frac{c^2}{36}; & r_7^2 &= \frac{4b^2}{9} + \frac{c^2}{36} \\ r_4^2 &= \frac{b^2}{9} + \frac{c^2}{9}; & r_8^2 &= \frac{4b^2}{9} + \frac{c^2}{9} \end{aligned}\right\} \quad \ldots \quad (3, 3)$$

Each calcium ion is surrounded by 6 CO_3 ions projecting on the plane $z = 0$ into an isosceles triangle and another 6 CO_3 ions projecting into a larger isosceles triangle. The distances and the number of ions in the respective distances is the same as in (3, 3).

Besides, each calcium ion is surrounded by 14 calcium ions, of which 4 are at distance s_1, 2 at s_2 ; 2 at s_3 ; 4 at s_4 and 2 at s_5 ; and each CO_3 is surrounded by 14 CO_3 ions of which 2 are at s_3 and 4 at each of the distances s_6 ; s_7 and s_8 ; where the distances are given by :—

$$\left.\begin{aligned} s_1^2 &= \frac{a^2}{4} + \frac{b^2}{36} + \frac{c^2}{4}\,; & s_5^2 &= \frac{4b^2}{9} + \frac{c^2}{4} \\ s_2^2 &= \frac{b^2}{9} + \frac{c^2}{4}\,; & s_6^2 &= \frac{a^2}{4} + \frac{b^2}{4} + \frac{c^2}{36} \\ s_3^2 &= a^2\,; & s_7^2 &= \frac{a^2}{4} + \frac{b^2}{4} + \frac{c^2}{9} \\ s_4^2 &= \frac{a^2}{4} + \frac{b^2}{4}\,; & s_8^2 &= \frac{a^2}{4} + \frac{b^2}{4} + \frac{4c^2}{9} \end{aligned}\right\} \quad \cdots \quad (3,\ 4)$$

Hence the potential per unit cell, due to the repulsive forces is given by

$$V_\triangle = 8\, b_{1,2} \left\{ \frac{2}{r_1^n} + \frac{2}{r_2^n} + \frac{1}{r_3^n} + \frac{1}{r_4^n} + \frac{2}{r_5^n} + \frac{2}{r_6^n} + \frac{1}{r_7^n} + \frac{1}{r_8^n} \right.$$
$$\left. - k \left(\frac{2}{s_1^n} + \frac{1}{s_2^n} + \frac{2}{s_3^n} + \frac{2}{s_4^n} + \frac{1}{s_5^n} + \frac{2}{s_6^n} + \frac{2}{s_7^n} + \frac{2}{s_8^n} \right) \right\} \quad \cdots \quad (3,\ 5)$$

Expressing the lengths of these sides in terms of δ (I, 2, 22) and taking $n = 6\cdot32$ (I, Table III)

$$V_\triangle = \frac{8\, b_{1,2}}{\delta^{6\cdot32}} \left(447\cdot8 - k\ 80\cdot4\right) \quad \cdots \quad (3,\ 6)$$

Comparing this with (3, 1)

$$2\, \frac{\alpha\, e^2\, \delta^{5\cdot32}}{6\cdot32 \times \delta^{5\cdot32}} = 8\, \frac{b_{1,2}}{\delta^{6\cdot32}} \left(447\cdot8 - k\ 80\cdot4\right) \quad \cdots \quad (3,\ 7)$$

whence

$$b_{1,2} = \frac{\alpha\, e^2\, \delta^{5\cdot32}}{4 \times 6\cdot32\,(447\cdot8 - k\ 80\cdot4)} \quad \cdots \quad (3,\ 8)$$

Substituting this in (3, 5)

$$V_\triangle = \frac{2\,\alpha\, e^2\, \delta^{5\cdot32}}{6\cdot32\,(447\cdot8 - k\,80\cdot4)} \left\{ \frac{2}{r_1^n} + \frac{2}{r_2^n} + \frac{1}{r_3^n} + \frac{1}{r_4^n} + \frac{2}{r_5^n} + \frac{2}{r_6^n} + \frac{1}{r_7^n} + \frac{1}{r_8^n} \right.$$
$$\left. - k \left(\frac{2}{s_1^n} + \frac{1}{s_2^n} + \frac{2}{s_3^n} + \frac{2}{s_4^n} + \frac{1}{s_5^n} + \frac{2}{s_6^n} + \frac{2}{s_7^n} + \frac{2}{s_8^n} \right) \right\} \quad \cdots \quad (3,\ 9)$$

The potential per unit volume is

$$V = \frac{1}{\delta^3} V_\triangle \quad \cdots \quad (3,\ 10)$$

We take

$$c_{11}^{r} = \frac{1}{2}\frac{2a\, e^2\, \delta^{5\cdot 32}}{6\cdot 32\;(447\cdot 8 - k\; 80\cdot 4)\;\delta^3}$$

$$\left[\sum_{h=1}^{8}\left\{t\frac{\partial^2}{\partial x^2}\left(\frac{1}{r_h^{\,n}}\right)\right\} x_h^{\,2} - k\sum_{j=1}^{8}\left\{\frac{\partial^2}{\partial x^2}\left(\frac{1}{s_j^{\,n}}\right)\right\}x_j^{\,2}\right] \quad .. \; (3,\, 11)$$

and $$c_{2,2}^{r^\theta} = \frac{1}{2}\frac{2a\, e^2\, \delta^{5\cdot 32}}{6\cdot 32\;(447\cdot 8 - k\; 80\cdot 4)\;\delta^3}\times$$

$$\left[\sum_{h=1}^{8}\left\{t\frac{\partial^2}{\partial y^2_\theta}\left(\frac{1}{r_h^{\,n}}\right)\right\}y^2{}_{\theta h} - k\sum_{j=1}^{8}\left\{t\frac{\partial^2}{\partial y^2_\theta}\left(\frac{1}{s_j^{\,n}}\right)\right\} y^2{}_{\theta j}\right] \quad .. \; (3,\, 12)$$

where t is 1 or 2 according as in (3, 9) and x_h is the x-component of r_h, x_j the x-component of s_j and $y_{\theta,h}$ and $y_{\theta,j}$ are the y_θ components of r_h and s_j respectively.

The value of k is determined by comparison with the experimental value of c_{11}.

§4. *Evaluation of* k *and* $c_{22}^{r^\theta}$.

Carrying out the differentiation and then substituting the numerical values of the r's and s's and their x-components in terms of δ

$$c_{11}^{r} = \frac{ae^2}{\delta^4\;(447\cdot 8 - k\; 80\cdot 4)}\;(755\cdot 6 - k\; 85\cdot 6) \qquad .. \qquad .. \; (4,\, 1)$$

The value of c_{11}, as experimentally determined by W. Voigt,[3] is $1\cdot 6\times 10^{12}$ dynes/cm.^{2}

From (1, 9) and (2, 14)

$$c_{11}^{r} = 2\cdot 362\times 10^{12}\ \text{dynes/cm.}^2 \qquad .. \qquad .. \qquad .. \qquad .. \; (4,\, 2)$$

Substituting the numerical values and comparing (4, 1) and (4, 2)

$$2\cdot 362 = \frac{1\cdot 105}{447\cdot 8 - k\times 80\cdot 4}\;(755\cdot 6 - k\; 85\cdot 6) \qquad .. \qquad .. \; (4,\, 3)$$

whence $k = 2\cdot 36$ .. .. (4, 4)

From (3, 12) we get by numerical simplification

$$c^{r^\theta} = 1\cdot 756\times 10^{12}\ \text{dynes/cm.}^2 \;.. \qquad .. \qquad .. \qquad .. \; (4,\, 5)$$

whence from (1, 9) and (2, 15)

$$c_{22}^{\theta} = 1\cdot 148\times 10^{12}\ \text{dynes/cm.}^2 \qquad .. \qquad .. \qquad .. \qquad .. \; (4,\, 6)$$

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[3] W. Voigt, *Ann. de Phy.*, 1907, 24, 290.

§5. *Comparison with the Experimental Value.*

The value of the elasticity-constant in the direction Oy_θ is not directly determined. With the help of the transformation formula for the elasticity-constants[4] we get

$$c_{22}^{\theta} = c_{11} \sin^4\theta + c_{22} \cos^4\theta + 2 \cos^2\theta \sin^2\theta \, (c_{12} + 2\, c_{66}) \quad \ldots \quad \ldots \quad (5, 1)$$

Substituting the values of the elasticity-constants from W. Voigt's measurements and the values of the trigonometric terms derived from (1, 1), we get

$$c_{22}^{\theta} = 1 \cdot 021 \times 10^{12} \text{ dynes/cm.}^2 \quad \ldots \quad \ldots \quad \ldots \quad \ldots \quad (5, 2)$$

The agreement between the two values given in (4, 6) and (5, 2) is quite satisfactory.

I wish to express my thanks to Prof. M. Born for his guidance in this work.

Summary.

The elasticity-constant c_{jh} consists of two parts c_{jh}^{e}, due to the electro-static forces and c_{jh}^{r} due to the repulsive forces. Considering the crystal as built up of a system of parallel neutral planes, the electro-static part of the elasticity-constant in a direction perpendicular to the system of planes, can be determined by considering the action on any one of the system of planes, of a few of its adjoining planes on one of its sides. c_{11}^{e} and $c_{22}^{e\,\theta}$ are determined in this way. The nature of the repulsive forces is completely determined by the equilibrium condition and by comparison with the experimental value of c_{11}. The value of $c_{22}^{r\,\theta}$ is then determined. The theoretical and experimental values of c_{22}^{θ} are found to agree well.

[4] W. Voigt, *Lehrbuch der Kristallphysik*, §291, p. 595.