

The spectral width of the emitted radiation was investigated with a Fabry-Perot interferometer. In general, one or more sharp components were observed of spectral width  $\sim 6 \times 10^{-4}$  Å superimposed on a broader background (see Fig. 16). The fringe patterns were not, however, reproducible; that is, the number and relative intensity of the components changed in each photographic exposure.

### DISCUSSION

The variation in the behavior of stimulated emission in ruby can be explained on the basis of the discussion in Part I. It was asserted that badly strained crystals scatter the energy into many cavity modes and that from the curves presented there it was expected that a clearly defined threshold would not be present in such cases. This is corroborated by the fact that the rubies which exhibit the pronounced beam and spectral narrowing, when viewed with polarized light, appear to be less strained than the others.

Several theories to account for the oscillatory nature of the output based upon relaxation behavior have been

advanced.<sup>8,10</sup> There is, however, a possibility that some type of mode-hopping process is also taking place, since the frequency of the inverted transition is certainly being swept in time during the oscillation pulse due to temperature changes and also due to a time-varying magnetic field produced by the current flow in the helical flash tube. Moreover, it is difficult to explain the appearance of several extremely narrowed lines observed with the Fabry-Perot interferometer unless some sort of mode sweeping is invoked. Further experimental work is indicated before the characteristics of the emitted light can be fully understood.

### ACKNOWLEDGMENTS

The authors are indebted to R. C. Pastor and H. Kimura for the chemical analysis of the rubies, to J. Bernath and M. Himber for the fabrication of the ruby samples, and to C. R. Duncan for the electronic instrumentation. We have benefited from helpful discussions with G. Birnbaum, R. W. Hellwarth, and W. G. Wagner.

<sup>10</sup> R. W. Hellwarth, *Phys. Rev. Letters* **6**, 9 (1961).

## Lattice Dynamics of Alpha Uranium\*

D. O. VAN OSTENBURG

*Argonne National Laboratory, Argonne, Illinois*

(Received September 14, 1960; revised manuscript received December 27, 1960)

The method developed by Begbie and Born has been applied to alpha uranium, where equations are developed which give the macroscopic elastic constants in terms of the microscopic force constants. Interactions of an atom with its first through fourth nearest neighbors, which involve twelve atoms, are considered. Through symmetry considerations, nineteen atomic force constants enter into this force system. An independent determination of the force constants is required before a valid verification of the solutions can be made. However, using measured values of the nine elastic constants, two sets of force constants are evaluated, one based upon quasi-central forces and the other upon neglect of fourth nearest neighbors.

### I. INTRODUCTION

BEGBIE and Born<sup>1</sup> developed the so-called "method of long waves" in order to study the relationship between elastic constants and atomic force constants. In their development the atomistic equations of motion are expressed in terms of the second derivatives of the potential energy function with respect to atomic displacements. These derivatives termed the atomic force constants are general in the sense that no assumption is made regarding the form of the potential. The elastic constants are obtained in terms of these atomic force constants by comparing these atomistic equations

of motion with the elastic equations for a macroscopic medium.

The structure of alpha uranium can be described as a close-packed hexagonal lattice that has been distorted to orthorhombic symmetry. Choosing any particular atom as origin, it has two nearest, two second nearest, four third nearest, and four fourth nearest neighbors. The structure may be viewed as two interpenetrating side-centered orthorhombic lattices with a unit cell containing two atoms. Using symmetry considerations it is possible to study the interactions of an atom with its first through fourth nearest neighbors in terms of nineteen atomic force constants.

In what follows, we develop equations which express the nine elastic constants in terms of these nineteen

\* This work was carried out under the auspices of the U. S. Atomic Energy Commission.

<sup>1</sup> G. H. Begbie and M. Born, *Proc. Roy. Soc. (London)* **A188**, 179 (1947); G. H. Begbie, *Proc. Roy. Soc. (London)* **A188**, 189 (1947).

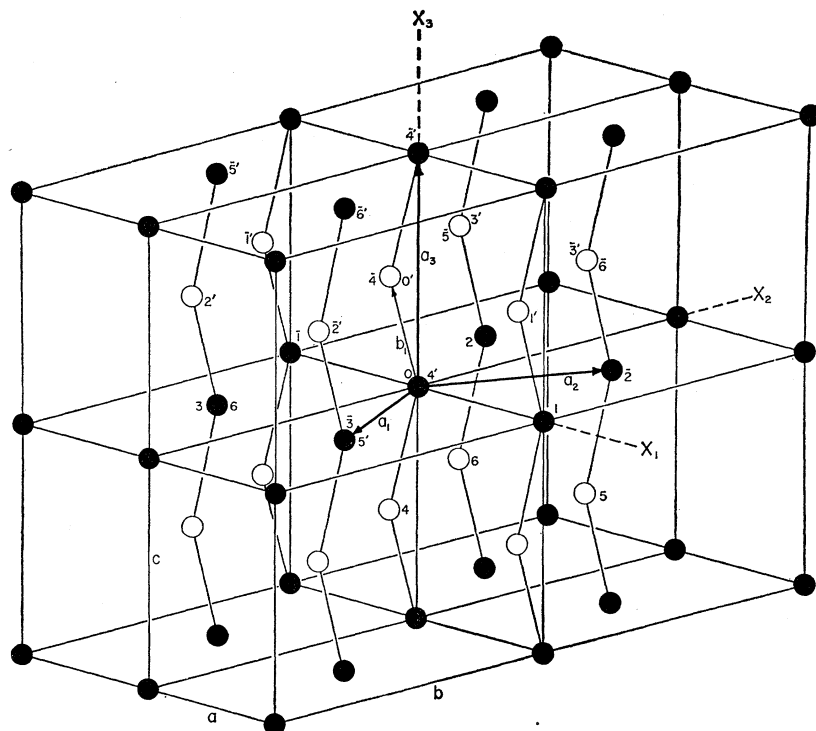


FIG. 1. First through fourth nearest neighbors of atoms  $O$  and  $O'$  of  $\alpha$  uranium. The unit cell is described by the basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , and  $\mathbf{a}_3$ . The vector  $\mathbf{b}_1$  separates the two interpenetrating lattices.

parameters. Using measured values<sup>2</sup> of the elastic constants of alpha uranium and certain assumptions, thirteen atomic force constants are evaluated for the case where fourth nearest neighbors are neglected. For the case of quasi-central forces between all atoms, fourteen force constants are computed. We must view these values merely as representing an order of magnitude. Before a more accurate test of the example can be made, an independent determination of the atomic force constants should be obtained.

## II. THEORY

The equilibrium position of an atom of type  $k$  in the  $l$ th cell is represented by the vector

$$\mathbf{r}(l; k) = \mathbf{r}(l) + \mathbf{r}(k),$$

where  $\mathbf{r}(l) = l_1 \mathbf{a}_1 + l_2 \mathbf{a}_2 + l_3 \mathbf{a}_3$ , with the  $l$ 's being integers;  $\mathbf{r}(k) = \lambda^1(k) \mathbf{a}_1 + \lambda^2(k) \mathbf{a}_2 + \lambda^3(k) \mathbf{a}_3$ , with  $0 \leq \lambda^i(k) < 1$  ( $i = 1, 2, 3$ ); and  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$  are the basis vectors of the unit cell.

For small displacements  $\mathbf{u}$  of atoms from their equilibrium positions, we can develop the potential energy of the lattice in a Taylor expansion. In the harmonic approximation, it is sufficient to retain only terms quadratic in the nuclear displacements. The coefficients of these terms we define as the negative of the atomic force constants. They have the form

$$\Phi_{\alpha\beta}(l-l'; kk') = \left[ \frac{\partial^2 \Phi}{\partial u_\alpha(l; k) \partial u_\beta(l'; k')} \right]_0. \quad (2.1)$$

In this expression  $\Phi$  is the lattice potential energy,  $u_\alpha(l; k)$  is the  $\alpha$  component of the displacement vector of lattice site  $(l; k)$ ,  $\alpha = 1, 2, 3$ , and  $u_\beta(l'; k')$  is the corresponding quantity for site  $(l'; k')$ .

The number of independent atomic force constants  $\Phi_{\alpha\beta}$  are reduced by observing the following: (1) The order of differentiation in (2.1) is immaterial, (2)  $\Phi$  is invariant under a rigid translation of the lattice as a whole, (3)  $\Phi$  is invariant under rotations, and (4)  $\Phi$  is invariant under all symmetry operations which belong to the space group of the crystal. These embody rotations, reflections, glide planes, and combinations of these. These statements are, respectively, manifested mathematically as

$$\Phi_{\alpha\beta}(l-l'; kk') = \Phi_{\beta\alpha}(l'-l; k'k), \quad (2.2)$$

$$\sum_{l'k'} \Phi_{\alpha\beta}(l-l'; kk') = 0, \quad (2.3)$$

$$\sum_{lk} \Phi_{\alpha\beta}(l-l'; kk') x_\lambda(l; k) = \sum_{lk} \Phi_{\lambda\beta}(l-l'; kk') x_\alpha(l; k), \quad (2.4)$$

and

$$\Phi(L-L'; KK') = \mathbf{T} \Phi(l-l'; kk') \mathbf{T}^{\text{tr}}, \quad (2.5)$$

where the matrix  $\mathbf{T}$  represents a symmetry operation of the lattice,  $\mathbf{T}^{\text{tr}}$  its transpose, and  $(L; K)$  is some other lattice position.

Using the method of long waves, as found in Born and Huang,<sup>3</sup> we relate the macroscopic elastic constants

<sup>2</sup> E. S. Fisher and H. J. McSkimin, *J. Appl. Phys.* **29**, 1473 (1958); H. J. McSkimin and E. S. Fisher, *ibid.* **31**, 1627 (1960).

<sup>3</sup> M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, New York, 1956), Chap. V.

to the interatomic force constants through the relation

$$c_{\alpha\gamma,\beta\lambda} = [\alpha\beta,\gamma\lambda] + [\beta\gamma,\alpha\lambda] - [\beta\lambda,\alpha\gamma] + (\alpha\gamma,\beta\lambda). \quad (2.6)$$

The square brackets are linear combinations of the atomic force constants and the curved brackets are linear combinations of products of the atomic force constants. Equation (2.6) holds only if we are dealing with a lattice initially free of stresses. The compatibility conditions for such a restriction are expressed in the additional relation

$$[\beta\gamma,\alpha\lambda] = [\alpha\lambda,\beta\gamma]. \quad (2.7)$$

In media free of stresses, the fourth-order tensor  $c_{\alpha\gamma,\beta\lambda}$  ( $\alpha, \gamma, \beta, \lambda = 1, 2, 3$ ) may be reduced to Voigt's notation  $c_{\rho\sigma}$  ( $\rho, \sigma = 1, \dots, 6$ ) in the usual manner.

### III. APPLICATION TO ALPHA URANIUM

Alpha uranium is orthorhombic with symmetry  $D_{2h}^{17}$ . Its structure is similar to the hexagonal metals except that atoms are skewed back and forth in the  $\langle 010 \rangle$  directions. The room temperature lattice constants are taken as  $a = 2.852$  Å,  $b = 5.865$  Å, and  $c = 4.945$  Å. The parameter  $\gamma$ , which is a measure of the skew behavior in the  $b$  direction, is taken as 0.105. With any particular atom as origin it has two nearest, two second nearest, four third nearest, and four fourth nearest neighbors. The structure may be regarded as a lattice with a basis in which there are two interpenetrating side-centered orthorhombic lattices with a unit cell containing two atoms. The unit cell is formed from the three basis vectors  $\mathbf{a}_1$ ,  $\mathbf{a}_2$ , and  $\mathbf{a}_3$ . The two interpenetrating lattices are separated by the basis vector  $\mathbf{b}_1$ . Figure 1 shows a portion of the lattice where we have labeled the twenty-four atoms involved in the calculation.

The twelve neighbors of origin  $O$  are split into two groups  $P$ ,  $\bar{P}$ , and those of  $O'$  into  $P'$ ,  $\bar{P}'$  as follows:

$$\begin{aligned} P &\rightarrow 1, 2, 3, 4, 5, 6; \\ \bar{P} &\rightarrow \bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{5}, \bar{6}; \\ P' &\rightarrow 1', 2', 3', 4', 5', 6'; \\ \bar{P}' &\rightarrow \bar{1}', \bar{2}', \bar{3}', \bar{4}', \bar{5}', \bar{6}'. \end{aligned}$$

The six atoms that are in the plane containing the origin  $O$  are denoted by type  $k=1$ , the six that lie in

the plane of  $O'$  are of type  $k=2$ , and so forth. The labeling procedure for convenience follows closely that of reference 1. It is convenient to reduce the indices ( $l; kk'$ ), representing the positions relative to the origin, to the notation  $(P; N)$ , where the correlation of ( $l; kk'$ )  $\rightarrow P$  is given in Table I, and  $N=1, 2, 3, 4$ , denotes the first, second, third, and fourth nearest neighbors, respectively. In this scheme  $D(l; kk') \rightarrow D(P; N)$ , where

$$D_{\alpha\beta}(l; kk') = [1/(m_k m_{k'})^{\frac{1}{2}}] \Phi_{\alpha\beta}(l; kk').$$

The symmetry operations of the lattice are referred to a Cartesian coordinate system centered at atom  $O$  and oriented as shown in Fig. 1. The symbol  $C_{2/m}^{2/c} 2_1/m$  describes the type of symmetry axes, etc. The symmetry operations which are sufficient to reduce the number of independent atomic force constants are as follows:

(a) A twofold axis of rotation about the  $x$  axis, followed by a reflection perpendicular to this axis and then a translation of amount  $(0, -2yb, \frac{1}{2}c)$ :

$$T_1 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \quad (3.1)$$

The corresponding change of label is

$$P \rightarrow \bar{P}' \quad \text{and} \quad P' \rightarrow \bar{P}.$$

It is to be noted that the translations affect only the change of label.

(b) A reflection in the plane perpendicular to the  $y$  axis plus a translation  $(0, -2yb, \frac{1}{2}c)$ :

$$T_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad P \rightarrow P', \quad \bar{P} \rightarrow \bar{P}'. \quad (3.2)$$

(c) A reflection in the plane perpendicular to the  $x$  axis:

$$T_3 = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (3.3)$$

$$1 \rightarrow \bar{1}, \quad 2 \rightarrow \bar{2}, \quad 3 \rightarrow \bar{3}, \quad 4 \rightarrow 4, \quad 5 \rightarrow 6, \quad 6 \rightarrow 5.$$

TABLE I. Atom positions referred to the basis vectors of the unit cell.

$P$	1	2	3	4	5	6	$\bar{1}$	$\bar{2}$	$\bar{3}$	$\bar{4}$	$\bar{5}$	$\bar{6}$
$l_1$	1	-1	0	0	0	-1	-1	0	1	0	-1	0
$l_2$	1	0	-1	0	1	0	-1	1	0	0	0	1
$l_3$	0	0	0	-1	-1	-1	0	0	0	0	0	0
$(kk')$	(11)	(11)	(11)	(21)	(21)	(21)	(11)	(11)	(11)	(21)	(21)	(21)
$P$	1'	2'	3'	4'	5'	6'	1'	2'	3'	4'	5'	6'
$l_1$	1	0	-1	0	1	0	-1	1	0	0	0	1
$l_2$	1	-1	0	0	0	-1	-1	0	1	0	-1	0
$l_3$	0	0	0	0	0	0	0	0	0	1	1	1
$(kk')$	(22)	(22)	(22)	(12)	(12)	(12)	(22)	(22)	(22)	(12)	(12)	(12)

TABLE II. Atomic force constant matrices for the origin nuclei and their first through fourth nearest neighbors.

$D(1; 2) \left\{ \begin{array}{l} -1 \\ D(\bar{1}; 2) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(2) & \delta(2) & 0 \\ -\delta(2) & \gamma(2) & 0 \\ 0 & 0 & \alpha(2) \end{pmatrix}$	$D(\bar{1}; 2) \left\{ \begin{array}{l} -1 \\ D(1'; 2) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(2) & -\delta(2) & 0 \\ \delta(2) & \gamma(2) & 0 \\ 0 & 0 & \alpha(2) \end{pmatrix}$
$D(2; 3) \left\{ \begin{array}{l} -1 \\ D(\bar{2}; 3) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(3) & \delta(3) & 0 \\ \epsilon(3) & \gamma(3) & 0 \\ 0 & 0 & \alpha(3) \end{pmatrix}$	$D(\bar{2}; 3) \left\{ \begin{array}{l} -1 \\ D(2'; 3) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(3) & -\delta(3) & 0 \\ -\epsilon(3) & \gamma(3) & 0 \\ 0 & 0 & \alpha(3) \end{pmatrix}$
$D(3; 3) \left\{ \begin{array}{l} -1 \\ D(\bar{3}; 3) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(3) & -\epsilon(3) & 0 \\ -\delta(3) & \gamma(3) & 0 \\ 0 & 0 & \alpha(3) \end{pmatrix}$	$D(\bar{3}; 3) \left\{ \begin{array}{l} -1 \\ D(3'; 3) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(3) & \epsilon(3) & 0 \\ \delta(3) & \gamma(3) & 0 \\ 0 & 0 & \alpha(3) \end{pmatrix}$
$D(4; 1) \left\{ \begin{array}{l} -1 \\ D(\bar{4}; 1) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(1) & 0 & 0 \\ 0 & \gamma(1) & \mu(1) \\ 0 & \mu(1) & \alpha(1) \end{pmatrix}$	$D(\bar{4}; 1) \left\{ \begin{array}{l} -1 \\ D(4'; 1) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(1) & 0 & 0 \\ 0 & \gamma(1) & -\mu(1) \\ 0 & -\mu(1) & \alpha(1) \end{pmatrix}$
$D(5; 4) \left\{ \begin{array}{l} -1 \\ D(\bar{5}; 4) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(4) & \delta(4) & \lambda(4) \\ \delta(4) & \gamma(4) & \mu(4) \\ \lambda(4) & \mu(4) & \alpha(4) \end{pmatrix}$	$D(\bar{5}; 4) \left\{ \begin{array}{l} -1 \\ D(5'; 4) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(4) & -\delta(4) & \lambda(4) \\ -\delta(4) & \gamma(4) & -\mu(4) \\ \lambda(4) & -\mu(4) & \alpha(4) \end{pmatrix}$
$D(6; 4) \left\{ \begin{array}{l} -1 \\ D(\bar{6}; 4) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(4) & -\delta(4) & -\lambda(4) \\ -\delta(4) & \gamma(4) & \mu(4) \\ -\lambda(4) & \mu(4) & \alpha(4) \end{pmatrix}$	$D(\bar{6}; 4) \left\{ \begin{array}{l} -1 \\ D(6'; 4) \end{array} \right\} = \frac{1}{m} \begin{pmatrix} \beta(4) & \delta(4) & -\lambda(4) \\ \delta(4) & \gamma(4) & -\mu(4) \\ -\lambda(4) & -\mu(4) & \alpha(4) \end{pmatrix}$
$D(O) \left\{ \begin{array}{l} -1 \\ D(O') \end{array} \right\} = \frac{1}{m} \begin{pmatrix} 2\beta(2)+4\beta(3)+2\beta(1)+4\beta(4) & 0 & 0 \\ 0 & 2\gamma(2)+4\gamma(3)+2\gamma(1)+4\gamma(4) & 0 \\ 0 & 0 & 2\alpha(2)+4\alpha(3)+2\alpha(1)+4\alpha(4) \end{pmatrix}$	

(d) A reflection in the plane perpendicular to the  $z$  axis:

$$T_4 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \begin{array}{lll} 1 \rightarrow \bar{1}, & 2 \rightarrow \bar{2}, & 3 \rightarrow \bar{3}, \\ 4 \rightarrow \bar{4}, & 5 \rightarrow \bar{6}, & 6 \rightarrow \bar{5}, \\ \bar{1} \rightarrow 1, & \bar{2} \rightarrow 2, & \bar{3} \rightarrow 3, \\ \bar{4} \rightarrow 4, & \bar{5} \rightarrow 6, & \bar{6} \rightarrow 5. \end{array} \quad (3.4)$$

(e) Equation (2.2) in connection with Table I gives us the identities,

$$\begin{aligned} D(1; 2) &= D^{\text{tr}}(\bar{1}; 2), & D(4; 1) &= D^{\text{tr}}(\bar{4}; 1), \\ D(2; 3) &= D^{\text{tr}}(\bar{3}; 3), & D(5; 4) &= D^{\text{tr}}(\bar{5}; 4), \\ D(3; 3) &= D^{\text{tr}}(\bar{2}; 3), & D(6; 4) &= D^{\text{tr}}(\bar{6}; 4), \\ D(1'; 2) &= D^{\text{tr}}(\bar{1}'; 2), & D(4'; 1) &= D^{\text{tr}}(\bar{4}'; 1), \\ D(2'; 3) &= D^{\text{tr}}(\bar{3}'; 3), & D(5'; 4) &= D^{\text{tr}}(\bar{5}'; 4), \\ D(3'; 3) &= D^{\text{tr}}(\bar{2}'; 3), & D(6'; 4) &= D^{\text{tr}}(\bar{6}'; 4). \end{aligned} \quad (3.5)$$

The use of Eq. (2.5) in conjunction with the stated symmetry operations gives us the dynamical matrices in their simplest form. From (3.1), we have

$$\begin{aligned} D(\bar{P}'; N) &= T_1 D(P; N) T_1^{\text{tr}} = D(P; N), \\ D(\bar{P}; N) &= T_1 D(P'; N) T_1^{\text{tr}} = D(P'; N). \end{aligned} \quad (3.6)$$

We see that we need only calculate the twelve matrices  $D(P; N)$  and  $D(\bar{P}; N)$  as the rest follow from (3.6).

The relations in (3.4) show for  $P=1, 2, 3, \bar{1}, \bar{2}, \bar{3}$ , that the atomic positions are not affected by  $T_4$ , and hence  $D(P; N) = T_4 D(P; N) T_4^{\text{tr}}$ . This gives  $D_{13}(P; 2) = D_{31}(P; 2) = D_{23}(P; 2) = D_{32}(P; 2) = 0$ . Now (3.3) takes  $1 \rightarrow \bar{1}, 2 \rightarrow \bar{2}$ , and  $3 \rightarrow \bar{3}$ . Using (3.3) and (3.5),

we find that  $D_{12}(1; 2) = D_{21}(\bar{1}; 2)$ ,  $D_{21}(1; 2) = D_{12}(\bar{1}; 2)$ , and so  $D_{12}(1; 2) = -D_{21}(1; 2)$ . Using these and the other symmetry operations, we get the structure of the remaining matrices.

The entire set of dynamical matrices is given in Table II, where  $D^O$  and  $D^{O'}$ , representing the force of the atoms  $O$  and  $O'$  on themselves, are determined from Eq. (2.3). In this table we have introduced Greek letters for the force constants where the arguments 1, 2, 3, 4, denote respectively the first, second, third, and fourth nearest neighbors.

The values of  $r^P$  to be used in Eqs. (2.6) are given in Table III.

Finally, through the use of Tables II and III and Eqs. (2.6), we arrive at the following equations giving the elastic moduli as functions of the atomic force constants:

$$c_{11} = \frac{2a}{bc} \left[ 2\beta(2) + \beta(3) + \beta(4) - \frac{4}{\Gamma(\gamma)} [2\delta(2) - \delta(3) + \epsilon(3) + 2\delta(4)]^2 \right], \quad (3.7)$$

$$c_{22} = \frac{2b}{ac} \left[ \gamma(3) + 8\gamma^2\gamma(1) + 4B^2\gamma(4) - \frac{64}{\Gamma(\gamma)} [\gamma\gamma(1) - B\gamma(4)]^2 \right], \quad (3.8)$$

$$c_{33} = \frac{2c}{ab} \left[ \frac{\alpha(1)}{2} + \alpha(4) - \frac{4}{\Gamma(\gamma)} [\mu(1) + 2\mu(4)]^2 \right], \quad (3.9)$$

TABLE III. Atom positions referred to the Cartesian coordinates centered at atom  $O$ .

$P$	1	2	3	$\bar{1}$	$\bar{2}$	$\bar{3}$	$P$	4	5	6	$\bar{4}$	$\bar{5}$	$\bar{6}$
$\frac{1}{a}x_1(l; 11)$	1	$-\frac{1}{2}$	$-\frac{1}{2}$	-1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{a}x_1(l; 21)$	0	$\frac{1}{2}$	$-\frac{1}{2}$	0	$-\frac{1}{2}$	$\frac{1}{2}$
$\frac{1}{b}x_2(l; 11)$	0	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{b}x_2(l; 21)$	$-2y$	$\frac{1}{2}-2y$	$\frac{1}{2}-2y$	$-2y$	$\frac{1}{2}-2y$	$\frac{1}{2}-2y$
$\frac{1}{c}x_3(l; 11)$	0	0	0	0	0	0	$\frac{1}{c}x_3(l; 21)$	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$

$$c_{66} = \frac{2b}{ac} \left[ \beta(3) + 8y^2\beta(1) + 4B^2\beta(4) - \frac{64}{\Gamma(\beta)} [y\beta(1) - B\beta(4)]^2 \right], \quad (3.10)$$

$$c_{55} = \frac{2a}{bc} [2\alpha(2) + \alpha(3) + \alpha(4)], \quad (3.11)$$

$$c_{44} = \frac{2c}{ab} \left[ \frac{1}{2}\gamma(1) + \gamma(4) - \frac{4}{\Gamma(\alpha)} [\mu(1) + 2\mu(4)]^2 \right], \quad (3.12)$$

$$c_{13} = \frac{4}{b} \left[ -\lambda(4) + \frac{2}{\Gamma(\gamma)} [\mu(1) + 2\mu(4)] [2\delta(2) - \delta(3) + \epsilon(3) + 2\delta(4)] \right] - \frac{2a}{bc} [2\alpha(2) + \alpha(3) + \alpha(4)], \quad (3.13)$$

$$c_{23} = \frac{8}{a} \left[ y\mu(1) - B\mu(4) - \frac{4}{\Gamma(\gamma)} [y\gamma(1) - B\gamma(4)] [\mu(1) + 2\mu(4)] \right] - \frac{2b}{ac} [\alpha(3) + 8y^2\alpha(1) + 4B^2\alpha(4)], \quad (3.14)$$

$$c_{12} = \frac{2}{c} \left[ -[\delta(3) + \epsilon(3)] + 4B\delta(4) + \frac{16}{\Gamma(\gamma)} [y\gamma(1) - B\gamma(4)] [2\delta(2) + \epsilon(3) - \delta(3) + 2\delta(4)] \right] - \frac{2a}{bc} [2\gamma(2) + \gamma(3) + \gamma(4)], \quad (3.15)$$

where  $\Gamma(\alpha) = 2\alpha(1) + 4\alpha(4)$ ,  $\Gamma(\beta) = 2\beta(1) + 4\beta(4)$ , and  $\Gamma(\gamma) = 2\gamma(1) + 4\gamma(4)$ .

The compatibility relation (2.7) and the invariance relations (2.4) give us additional relations among the force constants. Equation (2.7) gives

$$\begin{aligned} & \frac{2b}{ac} [\beta(3) + 8y^2\beta(1) + 4B^2\beta(4)] \\ &= \frac{2a}{bc} [2\gamma(2) + \gamma(3) + \gamma(4)], \quad (3.16) \end{aligned}$$

$$\frac{2a}{bc} [2\alpha(2) + \alpha(3) + \alpha(4)] = \frac{2c}{ab} [\frac{1}{2}\beta(1) + \beta(4)], \quad (3.17)$$

$$\frac{2b}{ac} [\alpha(3) + 8y^2\alpha(1) + 4B^2\alpha(4)] = \frac{2c}{ab} [\frac{1}{2}\gamma(1) + \gamma(4)], \quad (3.18)$$

while (2.4) gives

$$a[2\delta(2) + \epsilon(3) - \delta(3) - 2\delta(4)] = 4b[y\beta(1) - B\beta(4)], \quad (3.19)$$

$$4b[y\alpha(1) - B\alpha(4)] = c[\mu(1) + 2\mu(4)]. \quad (3.20)$$

We have a total of nineteen atomic force constants with fourteen relations between them. Equations (3.9) and (3.12) are equivalent to a single relation for our fourth nearest neighbor model, since their ratio equals  $\Gamma(\gamma)/\Gamma(\alpha)$ . This reduces the number of independent equations to thirteen.

#### IV. DISCUSSION

The model employed is based upon the fact that a solid is regarded as a collection of atoms coupled together by springs in which the spring constants play the role of the atomic bonds or atomic force constants. In view of this, the calculation expresses how the bond strengths and bond directions combine to give the various extensional and shear moduli. For example,  $c_{11}$  which is the extensional modulus in the  $x$  direction, depends upon atomic force constants of the second through fourth nearest neighbors. Intuitively, one expects a term relating the force in the  $x$  direction on the second nearest neighbor due to a unit displacement of the origin atom in the  $x$  direction. This is manifested through the appearance of  $\beta(2)$ . Similar arguments can be applied to the other linear terms appearing in this and the other elastic moduli.

Once the atomic force constants are known, we can determine the normal modes of vibration by solving the familiar secular equation and the frequency distribution spectrum determined. It turns out to be impossible to do this entirely from elastic constant data when considering interactions out to fourth nearest neighbors as the number of force constants exceed the number of equations. An independent determination of the atomic force constants is required before we can

proceed with such an evaluation. In principle it is possible to evaluate them according to various theoretical approaches<sup>4</sup> and/or to deduce them from experimental data obtained from long-wavelength neutron scattering.

For an order-of-magnitude evaluation of the atomic force constants, we have resorted to the quasi-central force approximation and the three nearest neighbor atom model. The elastic moduli  $c_{33}$  and  $c_{44}$  are each functions of the same argument. Consequently, the number of independent relations reduce to thirteen. The equation remaining serves as a cross check. In the numerical examples below the agreement with that equation was within an order of magnitude. It must also be noted that in the four nearest neighbor atom model,  $\delta(3)$ ,  $\epsilon(3)$ , and  $\delta(2)$  occur in such a way that all of them cannot be evaluated. This is a consequence of the fact that the matrices  $D(2;3)$  and  $D(3;3)$  are not symmetric. It is sufficient for them to be symmetric but not necessary. Therefore, in the calculation we have assumed  $\delta(3) = \epsilon(3)$ . This reduces the number of force constants to thirteen. The elastic moduli we obtained from extrapolations of the temperature-dependent data<sup>2</sup> to 0°K. The results are given in Table IV.

To achieve the quasi-central force parameters we set  $\beta(1)$ ,  $\gamma(2)$ ,  $\alpha(2)$ ,  $\delta(2)$ , and  $\alpha(3)$  equal to zero. The

TABLE IV. Elastic moduli in units of  $10^{12}$  dynes/cm<sup>2</sup> extrapolated to 0°K.

$c_{11} = 1.90$	$c_{66} = 0.865$
$c_{22} = 2.12$	$c_{12} = 0.387$
$c_{33} = 2.89$	$c_{23} = 1.099$
$c_{44} = 1.42$	$c_{13} = 0.255$
$c_{55} = 0.928$	

<sup>4</sup>H. C. White, Phys. Rev. **112**, 1092 (1958); A. B. Bhatia, *ibid.* **97**, 363 (1955).

TABLE V. Atomic force constants in units of  $10^4$  dynes/cm. Quasi-central atomic force constants.

$\gamma^*(1) = 10.1$	$\beta^*(3) = 2.6$	$\gamma^*(4) = -1.9$
$\alpha^*(1) = 7.7$	$\gamma^*(3) = 15.2$	$\alpha^*(4) = 4.7$
$\mu^*(1) = -2.5$	$\epsilon^*(3) = \delta^*(3) = 1.08$	$\delta^*(4) = 1.9$
$\beta^*(2) = 4.9$	$\beta^*(4) = 1.6$	$\lambda^*(4) = -3.3$
		$\mu^*(4) = -0.048$
Atomic force constants out to third-nearest neighbors.		
$\beta(1) = 3.1$	$\beta(2) = -4.5$	$\beta(3) = 1.9$
$\gamma(1) = -0.89$	$\gamma(2) = 3.4$	$\gamma(3) = 2.3$
$\alpha(1) = -5.7$	$\alpha(2) = 2.3$	$\alpha(3) = 0.19$
$\mu(1) = -2.8$	$\delta(2) = 1.4$	$\epsilon(3) = \delta(3) = -1.6$

remaining force constants are altered from the general situation and this fact is denoted by an asterisk. The term central force is reserved for two-body forces which interact only along the line joining their centers. The results of the quasi-central force approximation and the three nearest neighbor atom model are given in Table V. In each example there is a trend for the magnitudes to decrease as the neighbors become more distant, although the convergence is not rapid. Presumably, according to this model, atoms in alpha uranium possess long-range interactions. Their influence could be employed in the calculation by including fifth nearest and higher order neighbors and/or introducing a term into the equations of motion pertaining to the effects of the electron gas. However, in order to test the validity of such models, one would need data currently not available.

#### ACKNOWLEDGMENT

The author is indebted to E. S. Fisher for many helpful discussions and much encouragement throughout the course of the calculation.