reciprocal mass tensors reveals that the Fermi surface is disk shaped.

CONCLUSIONS

An ellipsoidal fit has been made to the Fermi surface of the new carriers. The fit is in all likelihood a distortion of the true surface. Analysis beyond the data given in Table I should await high-field dHvA measurements.

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Relation between Elastic Constants and Second- and Third-Order Force Constants for Face-Centered and Body-Centered Cubic Lattices

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The symmetry properties of a lattice are used to relate the second and third order force constants to the elastic constants of the lattice and to ascertain the number of independent force constants. Explicit relations are obtained for a face-centered cubic lattice with nearest neighbor interaction between atoms, and for a body-centered cubic lattice with nearest and next-nearest neighbor interactions. Corresponding relations are obtained for central forces in these two lattices.

I. INTRODUCTION

THE renewal of interest in the anharmonic properties of solids during the last few years draws attention to the problem of determining the force constants which appear in the theory of lattice dynamics. For the case of central forces, the interatomic potential can be characterized by two parameters, the well depth and the equilibrium interatomic separation. These are determined by measurement of the sublimation energy of the crystal and of its lattice spacing, respectively. The force constants are then obtained directly by differentiation of the interatomic potential with respect to the atomic separation. However, it has been shown[1] that a potential, such as the Mie–Lennard-Jones $(m,6)$ potential, does not give very good agreement with the experimental data available for the inert gas solids for any of the values $m=10$, 11, 12, 13, 14. The parameter m is a measure of the steepness of the repulsive part of the potential well. It has been suggested[1] that a third term might reasonably be added to the Mie–Lennard-Jones potential. If this term represents the dipole-quadrupole contribution to the van der Waals energy, the interatomic potential will have the form

$$\phi(r)=Ar^{-m}+Br^{-8}+Cr^{-6},$$

where r is the interatomic separation. Since there are now three parameters apart from m in the expression for $\phi(r)$, it is necessary to have experimental data in addition to that mentioned above in order to determine the third parameter. Though difficult to obtain in the case of the inert gas solids, the elastic constants are an obvious choice for this purpose. Therefore, it seems worthwhile to set forth here relations between the elastic constants and the force constants. Furthermore, in obtaining these relations we ascertain the number of independent force constants which arise in the lattice model under consideration.[2] This information is important when one is considering the possibility of extending a nearest neighbor, central force theory to noncentral forces, and further neighbors. It must be emphasized that the force constants are derivatives of the potential energy evaluated at the minimum of the potential energy, and that in the relations which we obtain, the elastic constants are also appropriate to the configuration which corresponds to the minimum of the potential energy. Since dynamic effects are excluded, the relations which we obtain correspond to elastic constants at the absolute zero of temperature in the approximation for which there is no zero-point motion. In order to determine these elastic constants from the experimental data, the zero-point energy of the lattice must be taken into account and the temperature dependence of the elastic constants must be determined. This problem will not be considered here.

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[1] G. K. Horton and J. W. Leech (to be published).

[2] The independent force constants for fcc and bcc lattices with nearest neighbor interaction have also been obtained by G. Leibfried and W. Ludwig in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1961), Vol. 12.

In Sec. II we summarize the work of Leibfried and Ludwig[3] and express the elastic constants in terms of combinations of the force constants which have the appropriate symmetry properties. In Sec. III we consider the case of a face-centered cubic lattice with nearest neighbor interaction and in Sec. IV we obtain the corresponding relations for the body-centered cubic lattice with nearest and next-nearest neighbor interaction between atoms. The special case of central forces in these two lattices is set forth in Sec. V.

II. GENERAL SYMMETRY CONSIDERATIONS

In this section we summarize the work of Leibfried and Ludwig[3] in which the restrictions imposed on the force constants by the requirements of symmetry are used to express the elastic constants in terms of appropriate combinations of force constants.

The energy density due to a homogeneous deformation v_{ik} is given by

$$u=\sum_{ik} C_{ik}V_{ik}+\frac{1}{2!}\sum_{ikjl} C_{ik,jl}V_{ik}V_{jl} +\frac{1}{3!}\sum_{ikjlrs} C_{ik,jl,rs}V_{ik}V_{jl}V_{rs}+\cdots, \quad (1)$$

where V_{ik} is defined by

$$2V_{ik}=v_{ik}+v_{ki}+\sum_{j=1}^{3} v_{ji}v_{jk},$$

and v_{ik} is defined by

$$r_i^{\mathbf{m}}=X_i^{\mathbf{m}}+\sum_{j=1}^{3} v_{ij}X_j^{\mathbf{m}},$$

$r_i^{\mathbf{m}}$ is the ith coordinate of the lattice point $\mathbf{m}$ and $X_i^{\mathbf{m}}$ is its mean position. Invariance of the energy density under rotation of the crystal is ensured since (V_{ik}) is zero for pure rotations.[4] The $C_{ik,jl,\cdots}$ are the elastic constants and are symmetric with respect to interchange of pairs of indices ik, jl, $\cdots$ and with respect to interchange of the members of a pair i, k.

In terms of the v_{ik}, Eq. (1) becomes

$$u=\sum_{ik} C_{ik}v_{ik}+\frac{1}{2!}\sum_{ikjl}[C_{ik,jl}+C_{kl}\delta_{ij}]v_{ik}v_{jl} +\frac{1}{3!}\sum_{ikjlrs}[C_{ik,jl,rs}+C_{ik,ls}\delta_{jr}+C_{ks,jl}\delta_{ir}+C_{kl,rs}\delta_{ij}] \times v_{ik}v_{jl}v_{rs}+\cdots. \quad (2)$$

When we expand the potential energy of the lattice $\Phi(\mathbf{r}^1,\mathbf{r}^2,\cdots\mathbf{r}^{\mathbf{m}},\cdots)$ in terms of the derivatives of the potential, we obtain

$$u=\frac{1}{V}(\Phi-\Phi_0) =\frac{1}{V}\Big\{\sum_{\mathbf{m},i}\Phi_i^{\mathbf{m}}q_i^{\mathbf{m}}+\frac{1}{2!}\sum_{\mathbf{m},\mathbf{n},i,j}\Phi_{ij}^{\mathbf{mn}}q_i^{\mathbf{m}}q_j^{\mathbf{n}} +\frac{1}{3!}\sum_{\mathbf{m},\mathbf{n},\mathbf{p},i,j,k}\Phi_{ijk}^{\mathbf{mnp}}q_i^{\mathbf{m}}q_j^{\mathbf{n}}q_k^{\mathbf{p}}+\cdots\Big\}, \quad (3)$$

where $\Phi_{ij\cdots}^{\mathbf{mn}\cdots}=\partial^\nu\Phi/\partial r_i^{\mathbf{m}}\partial r_j^{\mathbf{n}}\cdots$, the νth-order force constant is evaluated at the mean positions, $X_i^{\mathbf{m}}$, of the lattice points, V is the volume of the crystal and

$$q_i^{\mathbf{m}}=\sum_{j=1}^{3} v_{ij}X_j^{\mathbf{m}}.$$

We can define quantities $S_{ik,jl,\cdots}$ according to

$$S_{ik,jl,\cdots}=\frac{1}{V}\sum_{\mathbf{m},\mathbf{n},\cdots}\sum_{i,j,\cdots}\Phi_{ij\cdots}^{\mathbf{mn}\cdots}X_k^{\mathbf{m}}X_l^{\mathbf{n}}\cdots,$$

so that Eq. (3) becomes

$$u=\sum_{ik} S_{ik}v_{ik}+\frac{1}{2!}\sum_{ikjl} S_{ik,jl}v_{ik}v_{jl} +\frac{1}{3!}\sum_{ikjlrs} S_{ik,jl,rs}v_{ik}v_{jl}v_{rs}+\cdots. \quad (4)$$

By comparing Eqs. (2) and (4), we can express the $C_{ik,\cdots}$ in terms of the $S_{ik,\cdots}$. However, for a finite lattice the contribution to $S_{ik,\cdots}$ from points in the surface is of the same order as that from the interior points, so further constants $\hat{C}_{ij,\cdots}$ are introduced for which the surface effects are negligible. These constants are defined by

$$2\hat{C}_{ij,kl}=S_{ik,jl}+S_{il,jk} =\frac{1}{V}\sum_{\mathbf{mn}}\Phi_{ij}^{\mathbf{mn}}(X_k^{\mathbf{m}}-X_k^{\mathbf{n}})(X_l^{\mathbf{n}}-X_l^{\mathbf{m}}), \quad (5a)$$

and

$$2\hat{C}_{ij,rs,kl}=S_{ik,jl,rs}+S_{il,jk,rs} =\frac{1}{V}\sum_{\mathbf{mnp}}\Phi_{ijr}^{\mathbf{mnp}}(X_s^{\mathbf{p}}-X_s^{\mathbf{m}})(X_k^{\mathbf{m}}-X_k^{\mathbf{n}}) \times(X_l^{\mathbf{n}}-X_l^{\mathbf{m}}). \quad (5b)$$

For an ideal lattice, translational symmetry requires that

$$\Phi_{ij\cdots}^{\mathbf{mn}\cdots}=\Phi_{ij\cdots}^{\mathbf{m+h\ n+h}\cdots},$$

where $\mathbf{h}$ is a lattice vector, in which case the $\hat{C}_{ij,\cdots}$ depend on the relative separation of the lattice points. This means that the sums in Eqs. (5) can be carried out for an ideal lattice neglecting the contribution from points in the surface. Then Eqs. (5) become

$$2\hat{C}_{ij,kl}=-(1/V_z)\sum_{\mathbf{n}}\Phi_{ij}^{0\mathbf{n}}X_k^{\mathbf{n}}X_l^{\mathbf{n}}, \quad (6a)$$

[3] G. Leibfried and W. Ludwig, Z. Physik **160**, 80 (1960).
[4] G. Leibfried, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin and Göttingen, Heidelberg, 1955), Vol. VII/I, p. 238.

$$2\hat{C}_{ij,rs,kl}=-(1/V_z)\sum_{\mathbf{np}}\Phi_{ijr}{}^{0\mathbf{np}}X_s{}^{\mathbf{p}}X_k{}^{\mathbf{n}}X_l{}^{\mathbf{n}}, \quad (6b)$$

where V_z $(=V/N)$ is the volume per particle of the lattice.

Using Eqs. (2), (4), and (5) and the symmetry properties of the elastic constants we obtain the following relations:

$$C_{ik,jl}=\hat{C}_{ij,kl}+\hat{C}_{kj,il}-\hat{C}_{ik,jl}-C_{kl}\delta_{ij}-C_{il}\delta_{kj}+C_{jl}\delta_{ik}, \quad (7)$$

$$C_{ik,jl,rs}=\hat{C}_{ij,rs,kl}+\hat{C}_{kj,rs,il}-\hat{C}_{ik,rs,jl}-C_{kl,rs}\delta_{ij}-C_{il,rs}\delta_{kj}+C_{jl,rs}\delta_{ik}-\tfrac{1}{2}[2C_{ik,ls}+C_{il,ks}+C_{is,kl}]\delta_{jr}+\tfrac{1}{2}[C_{js,kl}-C_{jl,ks}]\delta_{ir}+\tfrac{1}{2}[C_{il,js}-C_{is,lj}]\delta_{kr}. \quad (8)$$

III. RELATIONS FOR THE FACE-CENTERED CUBIC LATTICE WITH NEAREST NEIGHBOR INTERACTION

First of all we need to know the independent force constants for the lattice model under consideration, namely, for a face-centered cubic lattice with nearest neighbor interaction.[2]

The second-order force constants are of two types, $\Phi_{ij}{}^{00}$ and $\Phi_{ij}{}^{0\mathbf{n}}$, where $\mathbf{n}$ is a nearest neighbor lattice point to the origin $\mathbf{0}$. When the independent components of $\Phi_{ij}{}^{0\mathbf{n}}$ have been obtained for one value of $\mathbf{n}$, all other $\Phi_{ij}{}^{0\mathbf{n}}$ are obtained by the appropriate symmetry operations which take $\mathbf{n}$ over all the nearest neighbor lattice points in a fcc lattice. Since the vector $\mathbf{0}$ is invariant with respect to interchange of $\pm x$, $\pm y$ and $\pm z$, the independent components of $\Phi_{ij}{}^{00}$ are easily obtained. The vector $\mathbf{n}=\mathbf{1}=(1,1,0)$ is invariant with respect to interchange of x and y and with respect to reflection in the x-y plane. These considerations yield the independent components of $\Phi_{ij}{}^{0\mathbf{n}}$. The results are given in Table I. The nearest neighbor vectors are expressed in units of $a_0/2$, where a_0 is the lattice parameter.

The restriction to nearest neighbors means that there are only three types of third-order force constant to consider,

$$\Phi_{ijk}{}^{000}, \quad \Phi_{ijk}{}^{00\mathbf{p}}, \quad \text{and} \quad \Phi_{ijk}{}^{0\mathbf{np}},$$

where $\mathbf{n}$ and $\mathbf{p}$ are nearest neighbors to the origin and to each other. The points $\mathbf{0}$, $\mathbf{n}$, $\mathbf{p}$ form an equilateral triangle which is typical of the close-packed structure therefore all other $\Phi_{ijk}{}^{0\mathbf{np}}$ are obtained by applying the appropriate symmetry operations to the original triangle. In order to obtain the independent components

TABLE I. Second-order force constants for fcc lattice.

n	$\Phi_{ij}{}^{0\mathbf{n}}$		
(0,0,0)	α_0	0	0
	0	α_0	0
	0	0	α_0
(1,1,0)	β_1	γ_1	0
	γ_1	β_1	0
	0	0	α_1

TABLE II. Third-order force constants for fcc lattice.

n	p	$\Phi_{xjk}{}^{0\mathbf{np}}$			$\Phi_{yjk}{}^{0\mathbf{np}}$			$\Phi_{zjk}{}^{0\mathbf{np}}$		
(0,0,0)	(1,1,0)	α_2	δ_2	0	β_2	β_2	0	0	0	γ_2
		β_2	β_2	0	δ_2	α_2	0	0	0	γ_2
		0	0	γ_2	0	0	γ_2	ϵ_2	ϵ_2	0
(1,0,1)	(1,1,0)	α_3	β_3	γ_3	ζ_3	$-\gamma_3$	η_3	ζ_3	δ_3	$-\zeta_3$
		γ_3	$-\beta_3$	δ_3	$-\zeta_3$	$-\alpha_3$	ζ_3	η_3	γ_3	ζ_3
		β_3	ϵ_3	$-\beta_3$	δ_3	β_3	γ_3	$-\gamma_3$	β_3	$-\alpha_3$

of the third-order force constants, one must use the symmetry properties of the $\Phi_{ij\cdots}{}^{\mathbf{mn}\cdots}$. It is clear from their definition in Eq. (3) that the $\Phi_{ij\cdots}{}^{\mathbf{mn}\cdots}$ possess the following properties:

$$\Phi_{ij\cdots}{}^{\mathbf{mn}\cdots}=\Phi_{ji\cdots}{}^{\mathbf{nm}\cdots}, \quad (9a)$$

$$\Phi_{ij\cdots}{}^{\mathbf{mn}\cdots}=(-1)^{\nu}\Phi_{ij\cdots}{}^{-\mathbf{m}\,-\mathbf{n}\cdots}, \quad (9b)$$

where ν is the order of the force constant. Also, they are invariant under translation by a lattice vector. These properties and the considerations which applied to the second-order force constants yield the independent components of $\Phi_{ijk}{}^{00\mathbf{p}}$ and $\Phi_{ijk}{}^{0\mathbf{np}}$. The results are given in Table II. It is immediately obvious from Eq. (9b) that $\Phi_{ijk}{}^{000}$ is zero.

We can reduce the number of independent constants still further by use of the relation which expresses translational invariance of the crystal as a whole, viz.,

$$\sum_{\mathbf{p}}\Phi_{ijk}{}^{0\mathbf{np}}=0, \quad (10)$$

and the requirement that the expression

$$\sum_{\mathbf{p}}\Phi_{ijk}{}^{0\mathbf{np}}X_r{}^{\mathbf{p}}+\Phi_{jk}{}^{0\mathbf{n}}\delta_{ir}+\Phi_{ik}{}^{0\mathbf{n}}\delta_{jr} \quad (11)$$

be symmetric in k, r, which is the condition for rotational invariance of the crystal as a whole.[3] From Eq. (10) we obtain

$$\sum_{\mathbf{p}}\Phi_{313}{}^{01\mathbf{p}}=\epsilon_2-\gamma_2+2(\beta_3-\gamma_3)=0, \quad (12)$$

and

$$\sum_{\mathbf{p}}\Phi_{212}{}^{01\mathbf{p}}=\delta_2-\beta_2+2(\beta_3-\zeta_3)=0. \quad (13)$$

The symmetry requirement Eq. (11) yields the following relations:

for $i=k=j=1$, $r=2$:

$$[-\alpha_2+\beta_2-2(\alpha_3+\gamma_3)]X_0=2\gamma_1, \quad (14)$$

for $i=k=1$, $j=r=3$:

$$[\epsilon_2+2\beta_3+2\gamma_3+2\zeta_3]X_0=\alpha_1-\beta_1, \quad (15)$$

for $i=1$, $k=2$, $j=r=3$:

$$[-\gamma_2+2\beta_3-2\delta_3-2\eta_3]X_0=\gamma_1 \quad (16)$$

where

$$a_0/2=X_0.$$

Thus there are seven independent third-order force constants.

Using the Voigt notation, the elastic constants for a lattice with cubic symmetry are c_{111}, c_{112}, c_{123}, c_{144}, c_{166}, and c_{456} which we can express according to Eqs. (7) and (8) as follows:

$$\begin{aligned} c_{111}&=\hat{C}_{11,11,11}-3c_{11},\\ c_{112}&=\hat{C}_{11,22,11}-c_{12},\\ c_{123}&=2\hat{C}_{12,33,12}-\hat{C}_{11,33,22}+c_{12},\\ c_{144}&=2\hat{C}_{12,23,13}-\hat{C}_{11,23,23}-c_{12},\\ c_{166}&=\hat{C}_{11,12,12}-c_{12}-2c_{66},\\ c_{456}&=\hat{C}_{33,12,12}-c_{66}, \end{aligned} \tag{17}$$

and

$$\begin{aligned} c_{11}&=\hat{C}_{11,11}-c_1,\\ c_{12}&=2\hat{C}_{12,12}-\hat{C}_{11,22}+c_1,\\ c_{44}&=\hat{C}_{22,33}-c_1. \end{aligned} \tag{18}$$

From Eq. (6a) and Table I we find that

$$\begin{aligned} -V_z\hat{C}_{11,11}&=4\beta_1X_0^2,\\ -V_z\hat{C}_{11,22}&=2(\alpha_1+\beta_1)X_0^2,\\ -V_z\hat{C}_{12,12}&=2\gamma_1X_0^2. \end{aligned} \tag{19}$$

The $\hat{C}_{ij,rs,kl}$ are obtained from Eq. (6b) and Table II and are as follows:

$$\begin{aligned} -V_z\hat{C}_{11,11,11}&=-4(\alpha_2-2\alpha_3)X_0^3,\\ -V_z\hat{C}_{11,22,11}&=-2(\beta_2-4\beta_3+2\gamma_3)X_0^3,\\ -V_z\hat{C}_{12,33,12}&=4(\epsilon_3+\delta_3)X_0^3,\\ -V_z\hat{C}_{11,22,33}&=2(4\beta_3-2\zeta_3-\gamma_2)X_0^3,\\ -V_z\hat{C}_{11,12,12}&=-2(\alpha_2+2\alpha_3)X_0^3,\\ -V_z\hat{C}_{33,12,12}&=-2(\gamma_2-2\zeta_3)X_0^3,\\ -V_z\hat{C}_{12,23,13}&=-2(\epsilon_2-2\gamma_3)X_0^3. \end{aligned} \tag{20}$$

Thus, we can express the elastic constants in terms of the nearest neighbor force constants using Eqs. (17) to (20), and we obtain

$$\begin{aligned} -V_zc_{111}&=-4(\alpha_2-2\alpha_3)X_0^3-12\beta_1X_0^2-3V_zc_1,\\ -V_zc_{112}&=-2(\beta_2-4\beta_3+2\gamma_3)X_0^3\\ &\quad -2(2\gamma_1-\alpha_1-\beta_1)X_0^2+V_zc_1,\\ -V_zc_{123}&=[8(\epsilon_2+\delta_3)-2(4\beta_3-2\zeta_3-\gamma_2)]X_0^3\\ &\quad +2(2\gamma_1-\alpha_1-\beta_1)X_0^2-V_zc_1,\\ -V_zc_{144}&=2(4\beta_3-2\zeta_3-\gamma_2)X_0^3\\ &\quad -2(2\gamma_1-\alpha_1-\beta_1)X_0^2+V_zc_1,\\ -V_zc_{166}&=-2(\alpha_2+2\alpha_3)X_0^3\\ &\quad -2(2\gamma_1+\alpha_1+\beta_1)X_0^2-V_zc_1,\\ -V_zc_{456}&=-2(\gamma_2-2\zeta_3)X_0^3-2(\alpha_1+\beta_1)X_0^2-V_zc_1. \end{aligned} \tag{21}$$

The elastic constant c_1 is zero for vanishing external stresses.

TABLE III. Second-order force constants for bcc lattice.

n	$\Phi_{ij}{}^{0n}$
(1,1,1)	α_5 β_5 β_5 β_5 α_5 β_5 β_5 β_5 α_5
(2,0,0)	α_7 0 0 0 β_7 0 0 0 β_7

IV. RELATIONS FOR THE BODY-CENTERED CUBIC LATTICE WITH NEAREST AND NEXT-NEAREST NEIGHBOR INTERACTIONS

Since the body-centered cubic lattice is not a close-packed structure, we shall take into account next-nearest as well as nearest neighbor interactions between atoms.

There are two types of second-order force constant to consider,

$$\Phi_{ij}{}^{01} \quad \text{and} \quad \Phi_{ij}{}^{05},$$

where $\mathbf{1}=(1,1,1)$ and $\mathbf{5}=(2,0,0)$. The other $\Phi_{ij}{}^{0n}$ are obtained by the appropriate symmetry operations. The invariance of $\mathbf{1}$ with respect to interchange of x, y, and z yields the independent components of $\Phi_{ij}{}^{01}$. The independent components of $\Phi_{ij}{}^{05}$ are obtained by requiring invariance with respect to interchange of $\pm y$ and $\pm z$. These results are shown in Table III.

Similar considerations together with the symmetry properties of the $\Phi_{ij}\ldots{}^{mn\cdots}$ given in Eq. (9) yield the independent components of $\Phi_{ijk}{}^{001}$ and $\Phi_{ijk}{}^{005}$. The only other type of third-order force constant is $\Phi_{ijk}{}^{015}$. This is invariant with respect to interchange of y and z. Further restrictions on $\Phi_{ijk}{}^{015}$ are obtained by the requirement of translational symmetry, e.g.,

$$\Phi_{ijk}{}^{015}=\Phi_{ijk}{}^{-5\ 1-5\ 0}=D_{-x}[\Phi_{kji}{}^{015}],$$

where D_{-x} is the operator which changes x to $-x$. These results are shown in Table IV.

The number of independent constants is further reduced by use of the conditions given in Eqs. (10) and (11). Thus, Eq. (10) gives

$$\textstyle\sum_{\mathbf{p}}\Phi_{121}{}^{01\mathbf{p}}=\gamma_4-\beta_4-\alpha_8+\beta_8-\gamma_8-\eta_8+\zeta_8=0, \tag{22}$$

and

$$\textstyle\sum_{\mathbf{p}}\Phi_{122}{}^{05\mathbf{p}}=\beta_6-\gamma_6+4\gamma_8=0. \tag{23}$$

TABLE IV. Third-order force constants for bcc lattice.

n	p	$\Phi_{xjk}{}^{0np}$			$\Phi_{yjk}{}^{0np}$			$\Phi_{zjk}{}^{0np}$		
(0,0,0)	(1,1,1)	α_4 γ_4 γ_4 β_4 β_4 δ_4 β_4 δ_4 β_4			β_4 β_4 δ_4 γ_4 α_4 γ_4 δ_4 β_4 β_4			β_4 δ_4 β_4 δ_4 β_4 β_4 γ_4 γ_4 α_4		
(0,0,0)	(2,0,0)	α_6 0 0 0 β_6 0 0 0 β_6			0 β_6 0 γ_6 0 0 0 0 0			0 0 β_6 0 0 0 0 γ_6 0		
(1,1,1)	(2,0,0)	0 α_8 α_8 β_8 γ_8 δ_8 β_8 δ_8 γ_8			α_8 0 0 $-\gamma_8$ ϵ_8 η_8 $-\delta_8$ ζ_8 η_8			α_8 0 0 $-\delta_8$ η_8 ζ_8 $-\gamma_8$ η_8 ϵ_8		

The symmetry requirement given in Eq. (11) yields the following relations:

for $\mathbf{n}=\mathbf{1}$, $i=j=k=1$, $r=2$:

$$\beta_4-\alpha_4-3\alpha_8-\gamma_8+2\epsilon_8+\eta_8=2\beta_5X_0^{-1}; \tag{24}$$

for $\mathbf{n}=\mathbf{1}$, $i=k=1$, $j=2$, $r=3$:

$$-\beta_4+\delta_4-\alpha_8-\gamma_8-2\delta_8+\eta_8+2\zeta_8=\beta_5X_0^{-1}; \tag{25}$$

for $\mathbf{n}=\mathbf{5}$, $i=r=1$, $j=k=2$:

$$-2\gamma_6-4\alpha_8+4\gamma_8=(\alpha_7-\beta_7)X_0^{-1}. \tag{26}$$

Thus, there are nine independent third-order force constants. Using Eq. (6a), and Table III we obtain the following expressions for the $\hat{C}_{ij,kl}$:

$$\begin{aligned}
&-V_z\hat{C}_{11,11}=4(\alpha_5+\alpha_7)X_0^2,\\
&-V_z\hat{C}_{11,22}=4(\alpha_5+\beta_7)X_0^2,\\
&-V_z\hat{C}_{12,12}=4\beta_5X_0^2.
\end{aligned}$$

The elastic constants c_{ij} are then obtained from Eq. (18). We find that

$$\begin{aligned}
&-V_zc_{11}=4(\alpha_5+\alpha_7)X_0^2+V_zc_1,\\
&-V_zc_{12}=4(2\beta_5-\alpha_5-\beta_7)X_0^2-V_zc_1,\\
&-V_zc_{66}=4(\alpha_5+\beta_7)X_0^2+V_zc_1.
\end{aligned} \tag{27}$$

The third order $\hat{C}_{ij,rs,kl}$ are obtained from Eq. (6b), and Table IV, and are given by

$$\begin{aligned}
&-V_z\hat{C}_{11,11,11}=-4(\alpha_4+2\alpha_6+2\epsilon_8)X_0^3,\\
&-V_z\hat{C}_{11,22,11}=-4(\beta_4+\alpha_8-4\beta_8+3\gamma_8+\eta_8)X_0^3,\\
&-V_z\hat{C}_{12,33,12}=-4(\delta_4+4\delta_8)X_0^3,\\
&-V_z\hat{C}_{11,33,22}=-4(\beta_4+\alpha_8+3\gamma_8+\eta_8-4\zeta_8)X_0^3,\\
&-V_z\hat{C}_{11,12,12}=-4(\alpha_4-2\epsilon_8)X_0^3,\\
&-V_z\hat{C}_{33,12,12}=-4(\beta_4+\alpha_8-\gamma_8-3\eta_8)X_0^3.
\end{aligned} \tag{28}$$

Then, using Eqs. (17), (27), and (28), the following relations are obtained for the elastic constants c_{ijk}:

$$\begin{aligned}
-V_zc_{111}&=-4(\alpha_4+2\alpha_6+2\epsilon_8)X_0^3\\
&\quad-12(\alpha_5+\alpha_7)X_0^2-3V_zc_1,\\
-V_zc_{112}&=-4(\beta_4+\alpha_8-4\beta_8+3\gamma_8+\eta_8)X_0^3\\
&\quad-4(2\beta_5-\alpha_5-\beta_7)X_0^2+V_zc_1,\\
-V_zc_{123}&=-4(2\delta_4+8\delta_8-\beta_4-\alpha_8-3\gamma_8-\eta_8+4\zeta_8)X_0^3\\
&\quad+4(2\beta_5-\alpha_5-\beta_7)X_0^2-V_zc_1,\\
-V_zc_{144}&=-4(\beta_4+\alpha_8+3\gamma_8+\eta_8-4\zeta_8)X_0^3\\
&\quad-4(2\beta_5-\alpha_5-\beta_7)X_0^2+V_zc_1,\\
-V_zc_{166}&=-4(\alpha_4-2\epsilon_8)X_0^3\\
&\quad-4(2\beta_5+\alpha_5+\beta_7)X_0^2-V_zc_1,\\
-V_zc_{456}&=-4(\beta_4+\alpha_8-\gamma_8-3\eta_8)X_0^3\\
&\quad-4(\alpha_5+\beta_7)X_0^2-V_zc_1.
\end{aligned} \tag{29}$$

V. CENTRAL FORCES

For the case of central force interaction between atoms the number of independent force constants is considerably reduced. Since

$$\begin{aligned}
&\Phi=\tfrac{1}{2}\textstyle\sum_{\mathbf{mn}}\phi(|\mathbf{r}^{\mathbf{m}}-\mathbf{r}^{\mathbf{n}}|),\\
&\Phi_{ijk}{}^{\mathbf{mnp}}=\frac{\partial^3\phi(|r^{\mathbf{m}}-r^{\mathbf{n}}|)}{\partial X_i{}^{\mathbf{m}}\partial X_j{}^{\mathbf{n}}\partial X_k{}^{\mathbf{p}}}=0 \quad \text{if} \quad \mathbf{m}\neq\mathbf{n}\neq\mathbf{p}.
\end{aligned} \tag{30}$$

Thus, in the fcc lattice we have

$$\alpha_3=\beta_3=\gamma_3=\delta_3=\epsilon_3=\eta_3=\zeta_3=0, \tag{31}$$

and in the bcc lattice,

$$\alpha_8=\beta_8=\gamma_8=\delta_8=\epsilon_8=\eta_8=\zeta_8=0. \tag{32}$$

The force constants which remain are of the form

$$\begin{aligned}
\Phi_{ijk}{}^{00\mathbf{h}}&=X_i{}^{\mathbf{h}}X_j{}^{\mathbf{h}}X_k{}^{\mathbf{h}}\left(\frac{1}{r^3}\phi'''(r)-\frac{3}{r^4}\phi''(r)+\frac{3}{r^5}\phi'(r)\right)\\
&\quad+(X_i{}^{\mathbf{h}}\delta_{jk}+X_j{}^{\mathbf{h}}\delta_{ki}+X_k{}^{\mathbf{h}}\delta_{ij})\\
&\quad\times\left(\frac{1}{r^2}\phi''(r)-\frac{1}{r^3}\phi'(r)\right),
\end{aligned} \tag{33}$$

and

$$\Phi_{ij}{}^{0\mathbf{h}}=-X_i{}^{\mathbf{h}}X_j{}^{\mathbf{h}}\left(\frac{1}{r^2}\phi''(r)-\frac{1}{r^3}\phi'(r)\right)-\frac{1}{r}\phi'(r)\delta_{ij}, \tag{34}$$

where r is the length of the vector $\mathbf{h}$ and $\phi'(r)$, etc. are derivatives of $\phi(r)$ with respect to r.

Using Eq. (31), the elastic constants for the face-centered cubic lattice simplify to the following expressions:

$$\begin{aligned}
&-V_zc_{111}=-4\alpha_2X_0^3-12\beta_1X_0^2-3V_zc_1,\\
&-V_zc_{112}=-2\beta_2X_0^3-2(2\gamma_1-\alpha_1-\beta_1)X_0^2+V_zc_1,\\
&-V_zc_{123}=2\gamma_2X_0^3+2(2\gamma_1-\alpha_1-\beta_1)X_0^2-V_zc_1,\\
&-V_zc_{144}=-2\gamma_2X_0^3-2(2\gamma_1-\alpha_1-\beta_1)X_0^2+V_zc_1,\\
&-V_zc_{166}=-2\alpha_2X_0^3-2(2\gamma_1+\alpha_1+\beta_1)X_0^2-V_zc_1,\\
&-V_zc_{456}=-2\gamma_2X_0^3-2(\alpha_1+\beta_1)X_0^2-V_zc_1.
\end{aligned} \tag{35}$$

Also, from Eq. (16) we have

$$-\gamma_2X_0=\gamma_1;$$

therefore, we find that

$$c_{123}=c_{456}=-c_{144}.$$

Using Eqs. (33) and (34), the independent force constants are expressed in terms of the derivatives of $\phi(r)$ evaluated at $r=a_0/\sqrt{2}$ as follows:

$$\alpha_2=\frac{1}{2\sqrt{2}}\left[\phi'''(r)+\frac{3}{r}\left(\phi''(r)-\frac{1}{r}\phi'(r)\right)\right],$$

$$\beta_2=\frac{1}{2\sqrt{2}}\left[\phi'''(r)-\frac{1}{r}\left(\phi''(r)-\frac{1}{r}\phi'(r)\right)\right],$$

$$\gamma_2=\frac{1}{r\sqrt{2}}\left[\phi''(r)-\frac{1}{r}\phi'(r)\right],$$

$$\alpha_1=-\frac{1}{r}\phi'(r) \tag{36}$$

$$\beta_1=-\frac{1}{2}\left(\phi''(r)+\frac{1}{r}\phi'(r)\right),$$

$$\gamma_1=-\frac{1}{2}\left(\phi''(r)-\frac{1}{r}\phi'(r)\right).$$

Then substituting these expressions into Eqs. (35) and putting $-c_1=p$, the external pressure, we find that the elastic constants are related to the force constants of a fcc lattice with nearest neighbor central force interaction between atoms by

$$c_{111}=\frac{1}{\sqrt{2}}\left[\phi'''(r)-\frac{3}{r}\phi''(r)-\frac{9}{r^2}\phi'(r)\right]-3p,$$

$$c_{112}=\frac{1}{2\sqrt{2}}\left[\phi'''(r)-\frac{3}{r}\phi''(r)+\frac{11}{r^2}\phi'(r)\right]+p, \tag{37}$$

$$c_{166}=\frac{1}{2\sqrt{2}}\left[\phi'''(r)-\frac{3}{r}\phi''(r)-\frac{5}{r^2}\phi'(r)\right]-p,$$

$$c_{123}=-(4/r^2\sqrt{2})\phi'(r)-p.$$

In the body-centered cubic lattice, use of Eqs. (32) in Eqs. (29) yields

$$\begin{aligned}
-V_z c_{111}&=-4(\alpha_4+2\alpha_6)X_0^3-12(\alpha_5+\alpha_7)X_0^2-3V_z c_1,\\
-V_z c_{112}&=-4\beta_4 X_0^3-4(2\beta_5-\alpha_5-\beta_7)X_0^2+V_z c_1,\\
-V_z c_{123}&=-4(2\delta_4-\beta_4)X_0^3\\
&\quad+4(2\beta_5-\alpha_5-\beta_7)X_0^2-V_z c_1,\\
-V_z c_{144}&=-4\beta_4 X_0^3-4(2\beta_5-\alpha_5-\beta_7)X_0^2+V_z c_1,\\
-V_z c_{166}&=-4\alpha_4 X_0^3-4(2\beta_5+\alpha_5+\beta_7)X_0^2-V_z c_1,\\
-V_z c_{456}&=-4\beta_4 X_0^3-4(\alpha_5+\beta_7)X_0^2-V_z c_1,
\end{aligned} \tag{38}$$

and Eqs. (22)–(26) reduce to the following:

$$\begin{aligned}
\gamma_4&=\beta_4,\\
\gamma_6&=\beta_6,\\
(\beta_4-\alpha_4)X_0&=2\beta_5,\\
(\delta_4-\beta_4)X_0&=\beta_5,\\
-2\gamma_6 X_0&=\alpha_7-\beta_7.
\end{aligned} \tag{39}$$

Then we have

$$\begin{aligned}
c_{123}&=c_{456}=c_{166},\\
c_{112}&=c_{144}.
\end{aligned} \tag{40}$$

Using Eqs. (33) and (34) we obtain

$$\begin{aligned}
\alpha_4&=\left[\frac{1}{3\sqrt{3}}\phi'''(r)+\frac{2}{r\sqrt{3}}\left(\phi''(r)-\frac{1}{r}\phi'(r)\right)\right]_{r=r_1},\\
\beta_4&=[(1/3\sqrt{3})\phi'''(r)]_{r=r_1},\\
\alpha_5&=-\tfrac{1}{3}[\phi''(r)+(2/r)\phi'(r)]_{r=r_1},\\
\beta_5&=-\tfrac{1}{3}[\phi''(r)-(1/r)\phi'(r)]_{r=r_1},\\
\alpha_6&=[\phi'''(r)]_{r=r_2},\\
\beta_6&=[(1/r)\phi''(r)-(1/r^2)\phi'(r)]_{r=r_2},\\
\alpha_7&=-[\phi''(r)]_{r=r_2},\\
\beta_7&=-[(1/r)\phi'(r)]_{r=r_2},
\end{aligned} \tag{41}$$

where r_1 is the nearest neighbor separation and r_2 is the next-nearest neighbor separation. Finally, we express the elastic constants of the body-centered cubic lattice in terms of derivatives of the central potential as follows:

$$\begin{aligned}
c_{111}&=\frac{1}{3\sqrt{3}}\phi'''(r_1)-\frac{1}{\sqrt{3}r_1}\phi''(r_1)-\frac{8}{r_1^2\sqrt{3}}\phi'(r_1)\\
&\quad+2\phi'''(r_2)-\frac{6}{r_2}\phi''(r_2)-3p,\\
c_{112}&=\frac{1}{3\sqrt{3}}\phi'''(r_1)-\frac{1}{\sqrt{3}r_1}\phi''(r_1)\\
&\quad+\frac{4}{r_1^2\sqrt{3}}\phi'(r_1)+\frac{2}{r_2^2}\phi'(r_2)+p,\\
c_{123}&=\frac{1}{3\sqrt{3}}\phi'''(r_1)-\frac{1}{\sqrt{3}r_1}\phi''(r_1)\\
&\quad-\frac{2}{r_1^2\sqrt{3}}\phi'(r_1)-\frac{2}{r_2^2}\phi'(r_2)-p.
\end{aligned} \tag{42}$$