TWO ANGULAR FORCE MODELS
FOR THE LATTICE DYNAMICS
OF CUBIC METALS

by

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ABSTRACT

We have used two angular force models to investigate the lattice dynamical properties of some cubic metals. Each of these two models consists of central force interaction between a particle and each of its first and second neighbours. In addition the first model also has an angular force interaction between a particle and each of its first and second neighbours (treated in de Launay's article [12]), while the second model has an angular force interaction between a particle and two of its first and second neighbours (treated in the paper by Gazis et al. [24]). Each model involves two central and two angular force constants.

For the second model, we give an alternative derivation of the results obtained by Clark et al. [23] for the b.c.c. lattice.

We apply both models to copper, aluminum and nickel (f.c.c.). It is found that the second model gives reasonably good results, better than those provided by the first model.

For b.c.c. lattice, we find that the two models are equivalent to each other and equivalent to the second neighbour tensor-force model, as far as the frequency spectrum is concerned. We apply this model to sodium, tantalum, molybdenum, tungsten and iron. For those metals whose dispersion curves are not complicated (e.g. Na, Fe), the second neighbour tensor-force model can be used with fair success.
CHAPTER I

INTRODUCTION

In order to explain the variation of specific heats at constant volume with changes of temperature for different materials, Einstein [1], in 1907, proposed a model of solid which consists of atoms, vibrating independently with the same frequency about their own positions of equilibrium. Though this model provides only a qualitative agreement with the experimental variation of the specific heats with temperature, it still serves as a great milestone in the studies of solids.

In 1912, Debye [2] developed a model of solid which employs as a postulate that all the atoms in a solid are not vibrating independently, but instead, are coupled together and vibrate collectively. Only the normal modes of vibration are taken as the motion of the system in reality. This laid down the foundation of the modern lattice dynamic theory of solids. A Debye cut-off frequency was introduced artificially so that the total number of normal modes is equal to that of the degrees of freedom of the system.

In Debye's theory, a crystal is treated as a continuum which is not true in reality. On the experimental side it is found that, the Debye temperature is not a constant at low temperatures. Born and von Kármán [3], in 1912, proposed their famous model of solid which treats the crystal as a discrete lattice as it actually is. An artificial periodic boundary condition was introduced by Born ([4], p. 557), so that only those
solutions of the equations of motion, which satisfy this boundary condition are the normal modes of vibration.

The interactions between the particles are expressed in terms of the elastic constants when passing to the long-wave limit. This is a good method of obtaining the characteristics of some microscopic quantities in terms of their asymptotic behaviour.

Blackman [5], Montroll [6], Bowers and Rosenstock [7] applied this model to a two-dimensional lattice with central force interaction between a particle and each of its first and second neighbours.

Fine [8] applied this model to the body-centered cubic lattice and Leighton [9] to the face-centered cubic lattice. These models assume central force interaction between a particle and each of its first and second neighbours. Though their results agree qualitatively with experiment, their basic assumption of purely central force interaction leads to the Cauchy relation which is not obeyed in metals.

The subject of lattice dynamics has been reviewed in recent years by Blackman [10] Born and Huang [11], de Launay [12], Cochran [13] and Maradudin, Montroll and Weiss [14].

The most general force constant model is that proposed by Begbie and Born [15] in 1947, now known as the tensor-force model. Begbie [16] applied this model to the face-centered cubic and the close-packed hexagonal lattices. Curien [17] has used this model for the b.c.c. lattice;
simplified versions have been used by Singh and Bowers [18] and by Hendricks, Riser and Clark [19]. Squires [20,21] has given general equations for interactions out to \( n \) neighbours on this model. The number of force constants required for each shell of atoms for the tensor-force model for b.c.c. and f.c.c. lattices are shown in Table I.

Table 1. The number of force constants required for each shell of neighbours for the tensor-force model.

<table>
<thead>
<tr>
<th>Shells of neighbours</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>f.c.c.</td>
<td>3</td>
<td>2</td>
<td>4</td>
<td>3</td>
<td>4</td>
<td>2</td>
<td>6</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td>b.c.c.</td>
<td>2</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>4</td>
<td>4</td>
</tr>
</tbody>
</table>

In recent years several models have been proposed which make special assumption as to the type of forces involved. The number of force constants for each shell of neighbours in these models is often less than the corresponding number on the tensor force model. Three of these models are identified below.

1. Besides the central force, de Laurier [12] has discussed a second type of force which depends on the angle which the line joining the moving atoms
makes with the equilibrium position of the line; this type is called an "angular force".* The mechanical analogy is a rod connecting the particles, the rod being fastened at its ends to the equilibrium positions by springs perpendicular to the rod. This model uses two force constants for each shell of neighbours. It is referred to as the "Angular Force Model I" (AFM-I) in this thesis.

2. Recently Clark, Gazis and Wallis [23] have investigated the frequency spectra of b.c.c. lattices using a model in which interatomic forces include angular forces of the type introduced by Gazis, Herman and Wallis [24]. This model contains angular forces as well as central forces between nearest and next-nearest neighbours and has four force constants; it will be referred to as the "Angular Force Model II" (AFM-II).

3. Lehman, Wolfram and De Wames [25] have proposed an axially symmetric model for lattice dynamics of metals. The basis of the model is the assumption that the internal energy of the system can be obtained by simply adding up all the bond-stretching and axially symmetric bond-bending terms. Varshni and Shukla [26] have given a treatment of the axially symmetric model when interactions out to any neighbour are considered. This model has two force constants associated with each shell of neighbours.

In the present thesis we have carried out the following investigations:

1) A treatment of the f.c.c. and b.c.c. lattices according to AFM-I.

* Angular forces were first introduced in lattice dynamics by Born [22] in his treatment of the sodium metal.
2) An alternative derivation of the results of Clark et al. [23] for the b.c.c. lattice on AFM-II, and further the model has been applied to the f.c.c. lattice.

Since there are four force constants in each of the models and only three elastic constants, we use the experimental values of the frequency of a longitudinal phonon at the zone boundary in the [100] direction. In terms of these four quantities, we obtain the values of the four inter-particle force constants.

After a brief introduction in Chapter I, the Born-von Kármán theory is discussed in Chapter II. In Chapter III, the angular force model I is discussed and the secular equations for both b.c.c. and f.c.c. lattices are obtained, while in Chapter IV, we deal with the angular force model II.

The two models have been applied to obtain the dispersion curves, vibration spectra and Debye temperatures of copper, aluminum, nickel (f.c.c.) and sodium, tantalum, molybdenum, tungsten and iron (b.c.c.). The results are compared with the experimental values. These are presented in Chapter V and Chapter VI.
CHAPTER II

BORN-VON KÁRMÁN THEORY

In contrast to the continuum assumption of the Debye theory, in the Born-von Kármán theory [3], crystals are treated as a system of interacting particles. The essential features of the theory for a simple Bravais lattice are discussed below.

Consider a system of \((N + 1)\) (finite) identical particles with no constraint imposed on them. These particles are vibrating about their own equilibrium positions which are located at the lattice points of a lattice representing the crystal formed by the \((N + 1)\) particles. Each particle has a mass \(M\). The system has \(3(N + 1)\) degrees of freedom which are represented by \(3(N + 1)\) independent coordinates, \(g_1, g_2, \ldots, g_{3(N + 1)}\). In lattice dynamic theory, we are interested in small oscillations of the particles about their equilibrium positions, denoted by \(g_{01}, \ldots, g_{03(N+1)}\).

The deviations of the \(3(N+1)\) coordinates from equilibrium are denoted by \(\varepsilon_i\):

\[ g_i = g_{0i} + \varepsilon_i \quad (i = 1, \ldots, 3(N+1)) \quad (2.1) \]

[27]

As shown by Goldstein, the total potential energy, \(V\), of the
system can be expanded in a Taylor series about the equilibrium.

\[
V(g_1, \ldots, g_{3(N+1)}) = V(g_{01}, \ldots, g_{03(N+1)}) + \sum_{i=1}^{3(N+1)} \left( \frac{\partial V}{\partial g_i} \right)_0 \varepsilon_i + 1/2 \sum_{i,j=1}^{3(N+1)} \left( \frac{\partial^2 V}{\partial g_i \partial g_j} \right)_0 \varepsilon_i \varepsilon_j + S
\]  (2.2)

where S is a sum of infinite number of terms involving higher derivatives of V. \(V(g_{01}, \ldots, g_{03(N+1)})\), being arbitrary, is chosen equal to 0.

Moreover, \(\left( \frac{\partial V}{\partial g_i} \right)_0 = 0 \) \( (i = 1, \ldots, 3(N+1)) \)

Assuming that the temperature is low and the displacement of each particle is small in magnitude such that S is negligible in comparing with the sum

\[
1/2 \sum_{i,j=1}^{3(N+1)} \left( \frac{\partial^2 V}{\partial g_i \partial g_j} \right)_0 \varepsilon_i \varepsilon_j,
\]

we have,

\[
V = 1/2 \sum_{i,j=1}^{3(N+1)} \left( \frac{\partial^2 V}{\partial g_i \partial g_j} \right)_0 \varepsilon_i \varepsilon_j
\]

In terms of \( \varepsilon_1, \ldots, \varepsilon_{3(N+1)} \) by making use of (2.1)

\[
V = \frac{1}{2} \sum_{i,j=1}^{3(N+1)} \left( \frac{\partial^2 V}{\partial g_i \partial g_j} \right)_0 \varepsilon_i \varepsilon_j
\]  (2.3)
Total kinetic energy of the system,

\[ T = \frac{1}{2} M \sum_{i=1}^{3(N+1)} \dot{\epsilon}_i^2 \]  \hspace{1cm} (2.4)

where \( \dot{\epsilon}_i = \frac{d\epsilon_i}{dt} \)

Lagrangian of the system,

\[ L = T - V \]

\[ = \frac{1}{2} M \sum_{i=1}^{3(N+1)} \dot{\epsilon}_i^2 - \frac{1}{2} \sum_{i,j=1}^{3(N+1)} \left( \frac{\partial^2 V}{\partial \dot{\epsilon}_i \partial \dot{\epsilon}_j} \right)_0 \epsilon_i \epsilon_j \]  \hspace{1cm} (2.5)

The Lagrange's equations are

\[ M \ddot{\epsilon}_i + \sum_{j=1}^{3(N+1)} \left( \frac{\partial^2 V}{\partial \dot{\epsilon}_i \partial \dot{\epsilon}_j} \right)_0 \epsilon_j = 0 \hspace{1cm} (i=1, \ldots, 3(N+1)) \]  \hspace{1cm} (2.6)

We use the cartesian coordinates

\[ x_0, y_0, z_0, \ldots, x_n, y_n, z_n \] as the 3(N+1) independent coordinates.

With \( x_0, y_0, z_0, \ldots, x_n, y_n, z_n \) representing the deviations of the particles from equilibrium, the Lagrange's equations (2.6) becomes
\[ \text{M} \hat{u}_m + \sum_{n=0}^{N} \left[ \left( \frac{\partial^2 V}{\partial u_m \partial x_n} \right) x_n + \left( \frac{\partial^2 V}{\partial u_m \partial y_n} \right) y_n \right. \]
\[ \left. \left. + \left( \frac{\partial^2 V}{\partial u_m \partial z_n} \right) z_n \right] = 0 \]
\[ (u = x, y, z; \ m = 0, \ldots, N) \]  

(2.7)

In the following, we denote \( \left( \frac{\partial^2 V}{\partial u_m \partial v_n} \right) \) by \( V_{m,n}^{u,v} \) where

\[ u = x, y, z; \ v = x, y, z; \ m = 0, \ldots, N; \ n = 0, \ldots, N, \]

and all the summations will be taken from 0 to N, unless otherwise stated.

We have

\[ V_{m,n}^{u,v} \equiv V_{n,m}^{v,u} \]  

(2.8)

We use as a trial solution of (2.7), a plane wave function

\[ \Psi = \hat{\alpha}_1 e^{i(\hat{\alpha}_1 \hat{r} - \omega t)} \]

or

\[ x = \hat{a}_1 e^{i(\hat{a}_1 \hat{r} - \omega t)} \]

\[ y = \hat{a}_2 e^{i(\hat{a}_2 \hat{r} - \omega t)} \]

\[ z = \hat{a}_3 e^{i(\hat{a}_3 \hat{r} - \omega t)} \]
By substitution of (2.9) into (2.7), we obtain a set of 3(N+1)
equations:

\[-\omega^2 M a_1 + \sum_n V_{mn} \left( x^x_{mn} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} \right)
+ \sum_n V_{mn} \left( x^y_{mn} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} \right)
+ \sum_n V_{mn} \left( x^z_{mn} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} \right) = 0 (2.10)\]

and two similar equations for y and z for each value of m. Moreover, m takes all the values from 0 to N \((\mathbf{\bar{r}}_n\) is the equilibrium position of the particle n).

In order to have nontrivial solutions of \(A_1, A_2\) and \(A_3\), for each m, the determinant

\[
\sum_n V_{mn}^{x^x_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} - \omega^2 M \sum_n V_{mn}^{x^y_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} \sum_n V_{mn}^{x^z_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)}
\]

\[
\sum_n V_{mn}^{y^x_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} \sum_n V_{mn}^{y^y_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} \sum_n V_{mn}^{y^z_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)}
\]

\[
\sum_n V_{mn}^{z^x_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} \sum_n V_{mn}^{z^y_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} \sum_n V_{mn}^{z^z_{mn}} e^{i q \cdot (\mathbf{r}_n - \mathbf{r}_m)} - \omega^2 M
\]

\[= 0 \quad (2.11)\]

\((m \text{ runs from } 0 \text{ to } N)\)
Because the interatomic force in a crystal are essentially short range in comparison with the dimensions of the crystal, \( V \left( \begin{array}{c} u \\ m \\ n \end{array} \right) \) will be negligible for distant neighbours of a particle. Since, in general, \( N \) is very large (e.g. of the order of \( 10^{23} \)), for most particles which are located inside the crystal, their environment will be identical. For these particles, \( \sum_n V \left( \begin{array}{c} x \\ m \\ n \end{array} \right) \) for different values of \( m \) will be identical. This is also true for other values of \( \sum_n V \left( \begin{array}{c} u \\ m \\ n \end{array} \right) \) \( (u = x, y, z; \ v = x, y, z) \). Therefore, these particles will have the same equation (2.11). For those particles located near the surface of the crystal, they will have equation (2.11) different from those of the particles located well inside the specimen. Since these particles are small in number in comparison with the number of particles located well inside the specimen (it varies as \( 6N^{2/3}/N \), i.e. \( N^{-1/3} \) and is of the order of \( 0 \) when \( N \) is of the order of \( 10^{23} \)), we shall disregard their special equations. Therefore, we can assume that for all the \( N \) particles, we have the same equation (2.11) and, hence, the same \( \omega \), \( \mathbf{k} \) relationship and the same ratios of \( A_1 \), \( A_2 \) and \( A_3 \) for each value of \( \mathbf{r} \). This justifies the choice of the plane wave function (2.9) as a solution of all the \( 3(N+1) \) equations in (2.7).

We take the origin of our coordinate system on a lattice point located well inside the crystal. The particle whose equilibrium position is at this lattice point is called the particle 0. The equation obtained by putting \( m = 0, \ \mathbf{r}_m = 0 \) into (2.11) is the secular equation of the crystal,
\[\sum_{n} v_{o n}^{(x)} e^{i \mathbf{q} \cdot \mathbf{R}_n} - \omega_M^2 = 0\]

\[\sum_{n} v_{o n}^{(y)} e^{i \mathbf{q} \cdot \mathbf{R}_n} - \omega_M^2 = 0\]

\[\sum_{n} v_{o n}^{(z)} e^{i \mathbf{q} \cdot \mathbf{R}_n} - \omega_M^2 = 0\]

\[\sum_{n} v_{o n}^{(x)} e^{i \mathbf{q} \cdot \mathbf{R}_n} - \omega_M^2 = 0\]

\[\sum_{n} v_{o n}^{(y)} e^{i \mathbf{q} \cdot \mathbf{R}_n} - \omega_M^2 = 0\]

\[\sum_{n} v_{o n}^{(z)} e^{i \mathbf{q} \cdot \mathbf{R}_n} - \omega_M^2 = 0\]

\[(u = x, y, z; v = x, y, z; \text{ includes } n = 0)\]

\[(2.12)\]

1.e. \[\left| \sum_{n} v_{o n}^{(u v)} e^{i \mathbf{q} \cdot \mathbf{R}_n} - \omega_M^2 \delta_{uv} \right| = 0\]

\[(u = x, y, z; v = x, y, z;\]

\[\delta_{uv} = \begin{cases} 
1 & u = v \\
0 & u \neq v 
\end{cases}\]

\[(2.13)\]
If we put \( \mathbf{q} = 2\pi \mathbf{k} \), \( \Omega = 2\pi \omega \) into (2.13), it becomes

\[
\sum_n V_n^{(u \: v)} e^{12\pi i \mathbf{k} \cdot \mathbf{r}_n} - 4\pi^2 \nu \gamma M_{uv} = 0
\]

\( u = x, y, z; \quad v = x, y, z \) \hspace{1cm} (2.14)

All distinct physical motions of the lattice represented by (2.9) are taken into account when the values of \( \mathbf{k} \) are restricted to one reciprocal lattice cell (Born & Huang [11], p. 63 to 70).

The usual periodic boundary condition is imposed on the solutions (2.9) to give the normal modes of vibration of the crystal. \( \mathbf{k} \) is restricted to some discrete values. The total number of vibrational modes, with \( \mathbf{k} \) restricted to a reciprocal lattice cell, is exactly \( 3(N+1) \) which is equal to the total number of degrees of freedom in this system of \( (N+1) \) particles. Hence, plane waves with distinct wave vectors \( \mathbf{k} \) in the same reciprocal cell and satisfying the periodic boundary condition, do correspond to distinct normal modes of vibration. Also, an artificial maximum frequency such as that introduced by Debye, is not required. (See, e.g. Born & Huang [11], p. 45, 46, 70)

Remark 2.1 - Essentially, we are interested in particles located well inside the crystal. For these particles (e.g. particles \( n_1, n_2, n_3 \) and \( n_4 \)) because of symmetry of the lattice, the determinant in (2.13) is symmetrical and we have
\( V_{n_1 n_2}^{(u,v)} = V_{n_3 n_4}^{(u,v)} \) if \( \hat{R}_{n_1} = -\hat{R}_{n_2} = \hat{r}(\hat{R}_{n_3} - \hat{R}_{n_4}) \) \hspace{1cm} (2.15)

i.e., \( V_{m,n}^{(u,v)} \) depends on the separation of the lattice points only.

In particular,

\[
\begin{align*}
V_{o n_1}^{(u,v)} &= V_{o n_2}^{(u,v)} \\
= V_{n_1 o}^{(v,u)} &= V_{n_2 o}^{(v,u)} & \text{if } \hat{R}_{n_1} = -\hat{R}_{n_2}
\end{align*}
\] \hspace{1cm} (2.16)

In order to emphasize the fact expressed by equation (2.15), some authors prefer to use the notation \( V_{m,-n}^{(u,v)} \) or \( V_{m,-n}^{(u,v)} \) (see, e.g., Born & Huang [11], equation (6.12) or Smith [28], equation (21)). Because in what follows, we need only use \( V_{o n}^{(u,v)} \), we prefer to stick to the notation \( V_{m,n}^{(u,v)} \).

Moreover, it has been shown by Smith [28] (p. 213 to 215) that:

\[
(1) \sum_{n} V_{o n}^{(u,v)} = \sum_{n} V_{n o}^{(v,u)} = 0
\]

\[u = x, y, z; \ v = x, y, z\] \hspace{1cm} (2.17)

i.e., \( V_{o o}^{(v,u)} = -\sum_{n=1}^{N} V_{n o}^{(v,u)} \)

\[u = x, y, z; \ v = x, y, z\] \hspace{1cm} (2.18)
(ii) when \( q \to 0 \), \( \omega \to 0 \)

(iii) \( \omega^2 \) is an even function of \( \hat{q} \).

Remark 2.2 - For a given value of \( \hat{q} \), equation (2.12) will have six roots of \( \omega \). Out of these six roots, only those real roots do correspond to physical wave motion, and need to be considered.

Actually, in (2.9), only the real components of \( \hat{s} \) are considered as representing physical motion, i.e.,

\[
\hat{s} (\text{real}) = \hat{A} \cos (\hat{q}, \hat{r} - \omega t) \tag{2.19}
\]

Since \( \omega^2 \) is an even function of \( \hat{q} \) and if \( \omega_1 \) and \( -\omega_1 \) are two real roots for a given wave vector \( \hat{q}_0 \), they will also be two real roots of \( -\hat{q}_0 \). But the wave

\[
\hat{s} (\text{real}) = \hat{A}^+ \cos (\hat{q}_0, \hat{r} - (-\omega t_1) t) \\
= \hat{A} \cos ((-\hat{q}_0), \hat{r} - \omega t_1) 
\]

is actually the same as the wave with \( \hat{q} = -\hat{q}_0 \), \( \omega = \omega_1 \). Similarly, the wave with \( \hat{q} = -\hat{q}_0 \), \( \omega = -\omega_1 \) and the wave with \( \hat{q} = \hat{q}_0 \), \( \omega = \omega_1 \) are the same wave. Therefore, for equation (2.12), we need only consider the positive roots of \( \omega \).
CHAPTER III

ANGULAR FORCE MODEL I - DE LAUNAY

This model consists of a cubic lattice with a central force and an angular force interaction between a particle and each of its first and second neighbours. This angular force interaction is of the type discussed in de Launay's article [12], p. 248. The effects of the more distant neighbours are neglected.

We locate the origin of our cartesian coordinate system on a lattice point situated well inside the crystal. The particle vibrating about this lattice point is called particle 0.

In what follows, since we are dealing with b.c.c. and f.c.c. lattices, we denote the positions of a lattice point by

\[ \hat{\mathbf{R}}_{on} = \hat{\mathbf{R}}_n = \frac{a}{2} \hat{\mathbf{N}}_n \]  

(3.1)

where "a" is the length of one side of the cube.

In this notation, (2.14) becomes

\[ \left| \sum_{n} V(u \mathbf{v}) e^{i \mathbf{p} \cdot \hat{\mathbf{N}}_n} - 4\pi 2 v 2 M_{uv} \right| = 0 \]  

(3.2)

where
\[ \dot{p} = \pi \dot{k}; \]
\[ \dot{u} = x_z - y_z - z_z; \quad \dot{v} = x, y, z \]

We shall discuss the general properties of the central force interaction and the angular force interaction before we deal with specific lattices.

(a) Central force interaction -

Let the force constant representing the central force between the particle \( m \) and the particle \( n \) be \( a_{mn} \).

The potential energy of the system of \( (N+1) \) particles due to central forces,

\[ V_a = \frac{1}{2} \sum_{m=0}^{N} \sum_{n=0}^{N} \left[ \frac{1}{2} a_{mn} (r_{mn} - R_{mn})^2 \right] \quad (3.4) \]

where

\[ R_{mn} = \left| \vec{R}_{mn} \right| \]
\[ \vec{R}_{mn} = (x_n - x_m) \hat{i} + (y_n - y_m) \hat{j} + (z_n - z_m) \hat{k} \]
\[ = \frac{a_{mn}}{\pi} \vec{N}_{mn} \quad (3.5) \]

is the equilibrium position of the particle \( n \) referring to that of the particle \( m \).

\[ r_{mn}^2 = (x_n + x_m - x_n)^2 + (y_n + y_m - y_n)^2 + (z_n + z_m - z_n)^2 \quad (3.6) \]
For \( n \neq 0 \),

\[
\left( \frac{\partial^2 v}{\partial y_n \partial x_o} \right)_o = v_{\alpha(n_0)}^{(y,x)} = -a_{on} \frac{y_n x_n}{R_{nn}^2} = -\frac{a_{on}}{N_n^2} (\hat{\vdots}^\vdots (1,N_n) (1,N_n) \vdots) \tag{3.7}
\]

where \( \hat{\vdots}^\vdots \) is defined in (3.1) and \( N_n = \left| \hat{\vdots}^\vdots \right| \).

\[
V_{\alpha(n_0)}^{(y,x)} = \sum_{n=1}^{N} \alpha_{on} \frac{y_n x_n}{R_{nn}^2} \]

\[
= -\sum_{n=1}^{N} V_{\alpha(n_0)}^{(y,x)} \tag{3.8}
\]

and (2.17) is verified.

Similarly for \( n \neq 0 \),

\[
v_{\alpha(n_0)}^{(x,x)} = -a_{on} \frac{x_n^2}{R_{nn}^2} \]

\[
= -\frac{a_{on}}{N_n^2} (\hat{\vdots}^\vdots (1,N_n) (1,N_n) \vdots) \tag{3.9}
\]
\[ v_{a(\hat{x}, \hat{x})} = \sum_{n=1}^{N} \alpha_{on} \frac{X_n^2}{R_{on}^2} \]

\[ = - \sum_{n=1}^{N} v_{a(\hat{r}, \hat{r})} \quad (3.10) \]

and (2.17) is verified.

(b) Angular force interaction (the type discussed in de Launay’s article [12]):

We denote the angular force constant representing the angular force interaction between the particle \( m \) and the particle \( n \) by \( \sigma_{mn} \).

From de Launay’s article [12], p. 249, the displacement which is effective for the angular force constant \( \sigma_{mn} \) due to displacements \( \hat{s}_n \) and \( \hat{s}_m \) of the particle \( m \) and particle \( n \) respectively, is \( \hat{\zeta}_{mn} \times (\hat{s}_n - \hat{s}_m) \) where, \( \hat{\zeta}_{mn} = \frac{\hat{\nu}_{mn}}{|\hat{\nu}_{mn}|} \) is the unit vector from the particle \( m \) to the particle \( n \). \( (\hat{\nu}_{mn} \) is defined in (3.5)

\[ \hat{s}_n = x_n\hat{i} + y_n\hat{j} + z_n\hat{k} \]

The change in potential energy due to \( \hat{s}_m \) and \( \hat{s}_n \),

\[ v_{\sigma_{mn}} = \frac{1}{2} \sigma_{mn} \left[ \hat{\zeta}_{mn} \times (\hat{s}_n - \hat{s}_m) \right]^2 \quad (3.11) \]
Let \( V_\sigma \) be the change of the total potential energy (angular force portion) due to displacements of all the \((N+1)\) particles. We have, for \( n \neq 0 \),

\[
V_\sigma(y \ x) = \sigma_{on} \left[ \vec{\xi}_n \times \vec{j} \right] \left[ \vec{\xi}_n \times (-\vec{i}) \right]
\]

\[
= \frac{\sigma_{on}}{N_n} \left( \vec{j} \cdot \vec{N}_n \right) \left( \vec{i} \cdot \vec{N}_n \right)
\]

(3.12)

where \( \vec{N}_n \) is defined in (3.1) and \( N_n = |\vec{N}_n| \).

\[
V_\sigma(y \ x) = \sum_{n=1}^{N} \sigma_{on} \left[ \vec{\xi}_n \times (-\vec{j}) \right] \left[ \vec{\xi}_n \times (-\vec{i}) \right]
\]

\[
= - \sum_{n=1}^{N} V_\sigma(y \ x)
\]

(3.13)

(3.14)

(3.15)

and (2.17) is verified.

Similarly, for \( n \neq 0 \),

\[
V_\sigma(x \ x) = \sigma_{on} \left( \frac{\vec{i} \cdot \vec{N}_n}{N_n} \right)^2 - 1
\]

\[
V_\sigma(x \ x) = - \sum_{n=1}^{N} V_\sigma(x \ x)
\]

(3.16)

(3.17)

and (2.17) is verified.
(1) **Body-centered Cubic Lattice**

(See Fig. 4-2)

The central force constant between a particle and each of its first neighbours is denoted by \( a_1 \), while that between it and each of its second neighbours is denoted by \( a_2 \).

The angular force constant between a particle and each of its first neighbours is denoted by \( \eta_1 \), while that between it and each of its second neighbours is denoted by \( \eta_2 \).

The force equations required are given in de Launay's article [12], (equation (7.7)). We can obtain the secular equation by means of equation (3.2). But, for the purpose of illustration, we start from the first principles, following the approach used by de Launay.

The first neighbours of particle 0 are labelled 1, 2, ..., 8, and its second neighbours 9, 10, ..., 14. (Fig. 4-2).

With the displacement of the particle \( n \) denoted by \( \xi_n \), the equation of motion for the particle 0 are:

\[
M \ddot{x}_0 = \left\{ - (8 \eta_1 + 6 \eta_2) x_0 + \eta_1 \sum_{i=1}^{8} x_i + \eta_2 \sum_{i=9}^{14} x_i \right. \\
- \frac{a_1 - \eta_1}{3} (8x_0 - \sum_{i=1}^{8} x_i - \sum_{i=1}^{4} y_i + \sum_{i=5}^{8} y_i)
\]
\[-z_1 z_2 + z_3 + z_4 - z_5 - z_6 + z_7 + z_8\]

\[-(a_2 - \eta_2) \left(2x_o - x_9 - x_{10}\right)\]

and two similar equations for \(y\) and \(z\). By substituting the plane wave solution (2.9) into (3.18) and with \(\hat{q} = 2\pi k, \ast = 2\pi\nu\), we obtain

\[
\begin{bmatrix}
\frac{8}{3} (a_1 + 2\eta_1) (1 - c_j c_k c_l) + 4a_2 \left( s_j^2 + 4\eta_j (S_j^2 + S_k^2) \right) \\
-4\pi^2 \nu^2 M
\end{bmatrix}
\begin{bmatrix}
A_1 \\
A_2
\end{bmatrix}
\begin{bmatrix}
\frac{8}{3} (a_1 - \eta_1) S_j S_k C_l \\
+ \frac{8}{3} (a_1 - \eta_1) S_j C_k S_l \\
A_3 = 0
\end{bmatrix}
\]

(3.19)

and two corresponding equations for \(y\) and \(z\)

where \(c_j = \pi a_k j\)

\(S_j = \sin \pi a_k j\)

\(k_1, k_2\) and \(k_3\) are the components of \(\vec{k}\) in cartesian coordinates.

These lead to the secular equation

\[
\begin{vmatrix}
G_1 - 4\pi^2 \nu^2 M & H_{12} & H_{13} \\
H_{21} & G_2 - 4\pi^2 \nu^2 M & H_{23} \\
H_{31} & H_{32} & G_3 - 4\pi^2 \nu^2 M
\end{vmatrix}
= 0
\]

(3.20)
where

\[ G_1 = \frac{8}{3} (a_1 + 2\eta_1) (1-C_1C_2C_3) + 4a_2s_1^2 + 4\eta_2(s_2^2 + s_3^2) \]

\[ H_{12} = \frac{8}{3} (a_1 - \eta_1) s_1s_2C_3 \]

and the others can be obtained by circular permutations of the indices.

In the long-wave limit as \( k \to 0 \), the secular equation becomes

\[
\begin{vmatrix}
I_1 - 4\pi^2v^2M & J_{12} & J_{13} \\
J_{21} & I_2 - 4\pi^2v^2M & J_{23} \\
J_{31} & J_{32} & I_3 - 4\pi^2v^2M \\
\end{vmatrix} = 0
\] (3.21)

where

\[ I_1 = \frac{2}{a} (a_2 - \eta_2)k_1^2 + \frac{2}{a} \left( \frac{a_1 + 2\eta_1}{3} + \eta_2 \right)k^2 - \rho v^2 \]

\[ J_{1j} = \frac{4}{3a} (a_1 - \eta_1)k_1k_j \]

\[ \rho = \frac{2M}{a^3} \quad \text{(density of the crystal)} \]

This should be identical with the elasticity secular equation

(de Launay [12]: Equation (10.9))
\begin{align*}
(c_{11} - c_{44})k_1^2 + c_{44}k^2 - \rho v^2 & \quad (c_{12} + c_{44})k_1k_2 & \quad (c_{12} + c_{44})k_1k_3 \\
\hline
(c_{12} + c_{44})k_1k_2 & \quad (c_{11} - c_{44})k_2^2 + c_{44}k^2 - \rho v^2 & \quad (c_{12} + c_{44})k_2k_3 \\
\hline
(c_{12} + c_{44})k_1k_3 & \quad (c_{12} + c_{44})k_2k_3 & \quad (c_{11} - c_{44})k_3^2 + c_{44}k^2 - \rho v^2
\end{align*}

= 0

(3.22)
By comparing (3.21) and (3.22), we have the identities,

\[ 2 \left( \frac{\alpha_1 + 2\eta_1}{3} + \eta_2 \right) = a_c c_{44} \]  
(3.23)

\[ 2 (\alpha_2 - \eta_2) = c_{11} - c_{44} \]  
(3.24)

\[ \frac{4}{3} (\alpha_1 - \eta_1) = c_{12} + c_{44} \]  
(3.25)

( longitudinal)

In the [100] direction, the phonon frequency at the first Brillouin zone boundary (i.e. \( k_1 = 1/a \)) is given by

\[ \nu_b = \frac{2}{\pi} \left[ \frac{1}{3M} (\alpha_1 + 2\eta_1) \right]^{1/2} \]  
(3.26)

From equations (3.23) to (3.26),

\[ \alpha_1 = \frac{1}{2} a(c_{12} + c_{44}) + \frac{1}{4} \pi^2 \nu_b^2 M \]  
(3.27)

\[ \alpha_2 = \frac{1}{2} a c_{11} - \frac{1}{4} \pi^2 \nu_b^2 M \]  
(3.28)

\[ \eta_1 = -\frac{1}{4} a (c_{12} + c_{44}) + \frac{1}{4} \pi^2 \nu_b^2 M \]  
(3.29)

\[ \eta_2 = \frac{1}{2} a c_{44} - \frac{1}{4} \pi^2 \nu_b^2 M \]  
(3.30)

By substituting (3.27), (3.28), (3.29) and (3.30) into (3.20), we obtain
a secular equation

\[
\begin{vmatrix}
G_1 - 4\pi^2 v^2 M & H_{12} & H_{13} \\
H_{21} & G_2 - 4\pi^2 v^2 M & H_{23} \\
H_{31} & H_{32} & G_3 - 4\pi^2 v^2 M
\end{vmatrix} = 0
\] (3.31)

where

\[
G_1 = 2\pi^2 v^2 M (1 - C_1 C_2 C_3) + (2a c_{11} - \pi^2 v^2 M) S_1^2 + (2a c_{44} - \pi^2 v^2 M) (S_2^2 + S_3^2)
\]

\[
H_{12} = 2a (c_{12} + c_{44}) S_1 S_2 C_3.
\]

and the others can be obtained by circular permutations of the indices.

(2) **Face-centered Cubic Lattice**

(See Fig. 4-3)

The central force constant between a particle and each of its first neighbours is denoted by \(a_1\), while that between it and each of its second neighbours is denoted by \(a_2\).

The angular force constant between a particle and each of its first neighbours is denoted by \(c_1\), while that between it and each of its second neighbours is denoted by \(c_2\).

As a matter of illustration, in obtaining the secular equation
for this kind of lattice, we use equation (3.2). Since we only need to use terms of \( \left( \frac{\partial^2 v}{\partial u_o \partial v_n} \right) \), we can treat the potential energy due to the central force and angular force interactions separately.

(a) Central force \((a_1, a_2)\) interaction -

From (3.7) and (2.16), we have

\[
V_{a_\alpha \alpha^\prime \alpha^\prime^\prime} = \begin{cases} 
0 & (n=1, 2, 3, 4) \\
-\frac{a_1}{2^\alpha} & (n=5, 6) \\
\frac{a_1}{2^\alpha} & (n=7, 8) \\
0 & (n=9, 10, 11, 12) \\
0 & (n=13, 14, \ldots, 18) 
\end{cases} \tag{3.32}
\]

\[
\frac{a_1}{2^\alpha} \tag{3.33}
\]

\[
\frac{a_1}{2^\alpha} \tag{3.34}
\]

\[
0 \tag{3.35}
\]

\[
0 \tag{3.36}
\]

From (3.8)

\[
V_{a_\alpha \alpha^\prime \alpha^\prime^\prime} = 0 \tag{3.37}
\]

Since from (2.8),

\[
V_{m n}^{u v} = V_{n m}^{v u},
\]
we have

$$
\sum_{n} v_{a(0n)}^{x} e^{i \mathbf{p} \cdot \mathbf{N}_{n}} = 2a_{1} S_{1} S_{2}
$$

(3.38)

where $S_{1}, S_{2}$ are defined in (3.19). Similarly from (3.9), (2.16) and (3.10),

$$
v_{a(0n)}^{x} = \begin{cases} 
- \frac{1}{2} a_{1} & (n=1, 2, \ldots, 8) \\
0 & (n=9, 10, 11, 12) \\
-a_{2} & (n=13, 14) \\
0 & (n=15, 16, 17, 18) \\
4a_{1} + 2a_{2} & (n=0)
\end{cases}
$$

(3.39)

(3.40)

(3.41)

(3.42)

(3.43)

Making use of (2.8) and (3.39) to (3.43), we have

$$
\sum_{n} v_{a(0n)}^{x} e^{i \mathbf{p} \cdot \mathbf{N}_{n}} = 4a_{1} - 2a_{1} C_{1} (C_{2} + C_{3}) + 4a_{2} S_{1}^{2}
$$

(3.44)

where $C_{1}, S_{1}$ are defined in (3.19).

Equations (3.38) and (3.44) have also been obtained by de Launay ([12], equation (11.6)).

(b) Angular force $(a_{1}, a_{2})$ interaction -

Since (3.13) can be obtained from (3.7) by replacing $a_{on}$ with
the result obtained for the central forces, namely, equation (3.38), can be used to obtain the corresponding result for the angular forces. Therefore,

\[ \sum_n V_{(n\to n)}(x y) e^{i\hat{p} \cdot \hat{N}} = -2\sigma_1 \mathbf{S}_1 \mathbf{S}_2 \]  

(3.45)

From (3.16), (2.16) and (3.17),

\[ V_{(n\to n)}(x y) = \begin{cases} 
- \frac{1}{2} \sigma_1 & (n=1, 2, \ldots, 8) \\
- \sigma_1 & (n=9, 10, 11, 12) \\
0 & (n=13, 14) \\
- \sigma_2 & (n=15, 16, 17, 18) \\
8 \sigma_1 + 4\sigma_2 & (n=0) 
\end{cases} \]  

(3.46)  

(3.47)  

(3.48)  

(3.49)  

(3.50)

Making use of (2.8) and (3.46) to (3.50), we have

\[ \sum_n V_{(n\to n)}(x y) e^{i\hat{p} \cdot \hat{N}} \]

\[ = 8\sigma_1 - 2\sigma_1 C_1(C_2 + C_3) - 4\sigma_1 C_2 C_3 + 4\sigma_2 (S_2^2 + S_3^2) . \]  

(3.51)
Combination of $\sigma_1$, $\sigma_2$, $\sigma_1$, $\sigma_2$ - 

After substitution of (3.38), (3.44), (3.45) and (3.51) into (3.2), we have a secular equation

\[
\begin{vmatrix}
K_1 - 4\pi^2 v^2 M & L_{12} & L_{13} \\
L_{21} & K_2 - 4\pi^2 v^2 M & L_{23} \\
L_{31} & L_{32} & K_3 - 4\pi^2 v^2 M
\end{vmatrix} = 0
\] (3.52)

where

\[
K_1 = 4\alpha_1 + 8\sigma_1 - 2(\alpha_1 + \sigma_1) C_1 (C_2 + C_3) - 4\sigma_1 C_2 C_3 + 4\sigma_2 S_1^2 + 4\sigma_2 (S_2^2 + S_3^2)
\]

\[
L_{12} = 2(\alpha_1 - \sigma_1) S_1 S_2
\]

and the remainder can be obtained by circular permutations of the indices.

In the long-wave limit as $k \to 0$, with $\rho = 4M/a^3$, the secular equation obtained should be identical with the elasticity secular equation (3.22). Therefore, by comparison, we have

\[
2\alpha_1 - 2\sigma_1 = a c_{12} + a c_{44} \quad (3.53)
\]

\[
\alpha_1 + 4\sigma_2 - \sigma_1 - 4\sigma_2 = a c_{11} - a c_{44} \quad (3.54)
\]

\[
\alpha_1 + 3\sigma_1 + 4\sigma_2 = a c_{44} \quad (3.55)
\]

In the [100] direction, the phonon frequency at the first Brillouin
zone boundary (i.e., \(k_1 = 1/a\)) is given by

\[
v_b = \frac{1}{\pi} \left[ \frac{2}{M} (\alpha_1 + \sigma_1) \right]^{1/2}
\]

(3.56)

From (3.53) to (3.56), we have

\[
\alpha_1 = \frac{1}{4} a (c_{12} + c_{44}) + \frac{1}{4} \pi^2 v_b^2 M
\]

(3.57)

\[
\alpha_2 = \frac{1}{4} a c_{11} - \frac{1}{4} \pi^2 v_b^2 M
\]

(3.58)

\[
\sigma_1 = -\frac{1}{4} a (c_{12} + c_{44}) + \frac{1}{4} \pi^2 v_b^2 M
\]

(3.59)

\[
\sigma_2 = \frac{1}{8} a (c_{12} + 3 c_{44}) - \frac{1}{4} \pi^2 v_b^2 M
\]

(3.60)

By substituting (3.57), (3.58), (3.59) and (3.60) into (3.52), we obtain a secular equation

\[
\begin{vmatrix}
K_1 - 4\pi^2 v_b^2 M & L_{12} & L_{13} \\
L_{21} & K_2 - 4\pi^2 v_b^2 M & L_{23} \\
L_{31} & L_{32} & K_3 - 4\pi^2 v_b^2 M
\end{vmatrix} = 0
\]

(3.61)

where \(K_1 = -a (c_{12} + c_{44}) + 3\pi^2 v_b^2 M\)

\[-\pi^2 v_b^2 M c_1 (c_2 + c_3)\]
\[ + (a c_{12} + a c_{44} - \pi^2 v_b^2 M) C_2 C_3 \]

\[ + (a c_{11} - \pi^2 v_b^2 M) S_1^2 \]

\[ + \left( \frac{1}{2} a c_{12} + \frac{3}{2} a c_{44} - \pi^2 v_b^2 M \right) (S_2^2 + S_3^2) \]

\[ L_{12} = a (c_{12} + c_{44}) S_1 S_2 \]

and the others can be obtained by circular permutations of the indices.
CHAPTER IV

ANGULAR FORCE MODEL II

This model consists of central force between a particle and each of its first and second neighbours, as well as angular forces which depend on the changes of angles in the triangles formed by the particle and its first and second neighbours. This type of angular force has been used by Gazis et al. [24] and Clark et al. [23]. The effects of the more distant neighbours are neglected.

In what follows, the general properties of the central forces and the angular forces are discussed before dealing with specific lattices.

(a) Central force interaction -

This is the same as that used in the angular force model I. The properties of these forces are discussed in Chapter III.

(b) Angular force interaction -

There are two types of triangles in which we are interested. One is formed by a particle and two of its first neighbours, called type (1) triangles. The other is formed by a particle, one of its first neighbours and one of its second neighbours, called type (2) triangles. (A more detailed discussion of this point will be given when we deal with
specific lattices).

The changes in the angles of a triangle are obtained by comparing the triangle of the equilibrium positions of these particles with the projection of the triangle of these particles, onto the plane of their equilibrium positions.

Consider the triangle formed by three particles a, b and c (Fig. 4-1). Let A, B and C denote their equilibrium positions; \( \vec{a} \), \( \vec{b} \) and \( \vec{c} \) denote their small displacements.

\( \hat{n}_{A,B,C} \) is defined as a unit vector which is in the plane A, B, C and normal to the vector \( \vec{A}_B \). We are dealing with the angle \( \theta_A \) at A.

The convention for the direction of \( \hat{n}_{A,B,C} \) is that, when \( \hat{n}_{A,B,C} \) is applied to particle B, it reduces the angle \( \theta_A \). (From definition \( \hat{n}_{A,B,C} = \hat{n}_{B,A,C} \).) \( \vec{A}_B \) is the position vector of B relative to A and \( \vec{R}_{A,B} = \left| \vec{R}_{A,B} \right| \hat{w} \) denotes a unit vector normal to the plane \( A,B,C \) in a direction such that \( \hat{w} \times \hat{A}_B \) and \( \hat{w} \) form a right-handed system. The projection of the displacement \( \vec{s}_b \) on the plane \( A,B,C \),

\[
\vec{s}_{bp} = (\hat{w} \times \vec{s}_b) \times \hat{w}
\]

Since the displacement \( \vec{s}_b \) is small in magnitude, the effective change in the angle \( \theta_A \) (as far as the angular force is concerned) due to \( \vec{s}_b \)
Fig. 4-1. Angular Force.
\[
\begin{align*}
\theta_A &= -\frac{\hat{s}_{bp} \cdot \vec{n}_{A,B,C}}{R_{A,B}} \\
\theta_B &= -\frac{\hat{s}_b \cdot \vec{n}_{A,B,C}}{R_{A,B}}
\end{align*}
\] (4.2)

The change in the angle \( \theta_A \) due to the displacements \( \hat{s}_a, \hat{s}_b \) and \( \hat{s}_c \),

\[
\delta \theta_A = \frac{(\hat{s}_a - \hat{s}_b) \cdot \vec{n}_{A,B,C}}{R_{A,B}} + \frac{(\hat{s}_a - \hat{s}_c) \cdot \vec{n}_{A,C,B}}{R_{A,C}}
\] (4.3)

Similarly, \( \delta \theta_B \) and \( \delta \theta_C \) can be obtained. The change in the potential energy due to \( \delta \theta_A, \delta \theta_B \) and \( \delta \theta_C \),

\[
= \frac{1}{2} \gamma_A (\delta \theta_A)^2 + \frac{1}{2} \gamma_B (\delta \theta_B)^2 + \frac{1}{2} \gamma_C (\delta \theta_C)^2
\] (4.4)

where \( \gamma_A, \gamma_B \) and \( \gamma_C \) are the angular force constants associated with the angles \( \theta_A, \theta_B \) and \( \theta_C \) respectively.

(1) **Body-centered Cubic Lattice**

(See Fig. 4-2)

Clark et al. [23] have obtained the secular equation for the angular force model II for the b.c.c. lattice from first principles. In this paper, we obtain the same secular equation (equation (4.51)) by means of equation (3.2)
Fig. 4-2. The first and second neighbours of the particle 0 of the b.c.c. lattice.
Since we only need to use terms of \( \frac{\partial^2 V}{\partial u_o \partial V_n} \), we can treat the potential energy due to the central force interaction and the angular force interaction separately.

(a) Central force \((a_1, a_2)\) interaction -

The central force constant between a particle and each of its first neighbours is denoted by \(a_1\), while that between it and each of its second neighbours is denoted by \(a_2\). From (3.7), (2.16), (3.8) and (2.8), we have

\[
V_{a_{\alpha} (n \n o)} = \begin{cases} 
-\frac{a_1}{3} & (n=1, 2, 3, 4) \\
\frac{a_1}{3} & (n=5, 6, 7, 8) \\
0 & (n=9, 10, \ldots, 14) \\
0 & (n=0) 
\end{cases}
\]  

(4.5)  

(4.6)  

(4.7)  

(4.8)

and

\[
\sum_n V_{a_{\alpha} (n \n o)} e^{i p \cdot \vec{N}_n}
\]

\[
= \frac{8a_1}{3} S_1 S_2 S_3
\]

(4.9)
where \( S_1, C_1 \) are defined in (3.19). Similarly, from (3.9), (2.16),
(3.10) and (2.8), we have

\[
V_{\alpha n0}^{x x} = \begin{cases} 
-\frac{a_1}{3} & (n=1, 2, \ldots, 8) \\
-a_2 & (n=9, 10) \\
0 & (n=11, 12, 13, 14) \\
\frac{8a_1}{3} + 2a_2 & (n=0)
\end{cases}
\]  

(4.10)

(4.11)

(4.12)

(4.13)

and

\[
\sum_n V_{\alpha n0}^{x x} e^{ip \cdot \hat{N} n} = \frac{8a_1}{3} (1 - C_1 C_2 C_3) + 4a_2 S_1^2
\]

(4.14)

where \( C_1, S_1 \) are defined in (3.19). Equations (4.9) and (4.14) have
also been obtained by de Launay([12], equation (11.5))

(b) Angular force \((\mu_1, \mu_2)\) interaction -
(See Fig. 4-2)

There are two types of triangles which we are going to consider.
The first one is that formed by a particle and two of its first neighbours.
They are triangles equivalent to \( \Delta 0, 3, 8 \) in Fig. 4-2; particle 8 is a
second neighbour of particle 3. This type of triangles is called type (1) triangles.

The other one is that formed by a particle, one of its first neighbours and one of its second neighbours. They are triangles equivalent to Δ0, 3, 11; particle 11 is a first neighbour of particle 3. This type of triangles is called type (2) triangles.

There are, in all, twelve type (1) triangles and twenty-four type (2) triangles, referring to the particle 0. As shown in Fig. 4-2, all the thirty-six triangles are identical and each is isosceles with two equal angles $\theta_2$. We shall associate with each angle $\theta_1$ in the triangles an angular force constant $\nu_1$, and each angle $\theta_2$, an angular force constant $\nu_2$.

The unit normals $\hat{\hat{n}}_{A_2B_3}$ in (4.1) are given by

$$\hat{\hat{n}}_{1_0,1_0} = \frac{1}{\sqrt{3}} \left( \begin{array}{c} a \\ -\frac{a}{3} \end{array} \right)$$

(4.15)

$$\hat{\hat{n}}_{0_1} = \sqrt{\frac{3}{6}} \left( \hat{\hat{n}}_j - \frac{1}{3} \hat{\hat{n}}_i \right) = \hat{\hat{n}}_{0_1,1_0}$$

(4.16)

$$\hat{\hat{n}}_{1_0,1_0} = \frac{1}{\sqrt{2a}} \left( \hat{\hat{n}}_1 + \hat{\hat{n}}_j \right)$$

(4.17)
\[
\hat{n}_{1,m,o} = \frac{1}{\sqrt{\frac{8}{3}}} \begin{bmatrix} -\hat{N}_1 - e(\hat{N}_m - \hat{N}_i) \end{bmatrix} \frac{a}{2}
\]

\[
= -\frac{1}{\sqrt{2a}} (\hat{N}_m + 2\hat{N}_1) = \hat{n}_{m,1,o} \quad (4.18)
\]

\[
\hat{n}_{o,1,m} = \frac{1}{\sqrt{\frac{8}{3}}} \begin{bmatrix} (\hat{N}_m - \hat{N}_1) - e(-\hat{N}_1) \end{bmatrix} \frac{a}{2}
\]

\[
= \sqrt{\frac{3}{8}} (\hat{N}_m - \frac{2}{3} \hat{N}_1) = \hat{n}_{1,o,m} \quad (4.19)
\]

\[
\hat{n}_{m,o,1} = -\frac{1}{\sqrt{2a}} [ (\hat{N}_m - \hat{N}_1) + (-\hat{N}_1)] \frac{a}{2}
\]

\[
= \frac{1}{\sqrt{2}} (2\hat{N}_1 - \hat{N}_m) = \hat{n}_{o,m,1} \quad (4.20)
\]

where \[e = \frac{\hat{N}_k\hat{N}_r\hat{N}_t}{\hat{N}_k\hat{N}_r\hat{N}_t}\] (k, r, t form a type (1) triangle referring to particle k; k takes an appropriate value out of \(0, 1, 2, \ldots, 8\), \(4.21\))

\(i, j\) denote the first neighbours of particle 0, and \(m\) the second neighbours.
We shall deal with the potential energy corresponding to \( \mu_1 \) first, then that corresponding to \( \mu_2 \).

(1) Potential energy corresponding to \( \mu_1 \) —

\[
V_{\mu_1} = \frac{1}{2} \mu_1 \left\{ \frac{(\hat{s}_0 - \hat{s}_1) \cdot \hat{n}_{0,1,3}}{\sqrt{3} a} + \frac{(\hat{s}_0 - \hat{s}_3) \cdot \hat{n}_{0,3,1}}{\sqrt{3} a} \right\}^2
\]

(This is the contribution of the type (1) triangle 0, 1, 3)

+ \ldots (contribution of the twelve type (1) triangles referring to the particle 0)

\[
+ \left[ \frac{(\hat{s}_1 - \hat{s}_9) \cdot \hat{n}_{1,9,0}}{\sqrt{3} a} + \frac{(\hat{s}_1 - \hat{s}_0) \cdot \hat{n}_{1,0,2}}{\sqrt{3} a} \right]^2
\]

(This is the contribution of the type (2) triangle 0, 1, 9)

+ \ldots (contribution of the twenty-four type (2) triangles referring to the particle 0).

+ (contribution of all other triangles which do not involve the particle 0)

(4.22)

By substituting (4.16), (4.18), (4.19) into (4.22), we have

\[
V_{\mu_1} = \frac{\mu_1}{4a^2} \left\{ \left[ (\hat{s}_0 - \hat{s}_1) \cdot (\hat{n}_3 - \frac{1}{3} \hat{n}_1) + (\hat{s}_0 - \hat{s}_3) \cdot (\hat{n}_1 - \frac{1}{3} \hat{n}_3) \right]^2
\]

+ \ldots (contribution of the twelve type (1) triangles referring to the particle 0).
\[ + \frac{1}{3} (\hat{s}_1 - \hat{s}_0) \cdot (\hat{n}_9 + 2 \hat{n}_1) + (\hat{s}_1 - \hat{s}_0) \cdot (\hat{n}_9 - \frac{2}{3} \hat{n}_1) \] 
\[ + \ldots \quad \text{(contribution of the twenty-four type (2) triangles referring to the particle 0)} \]
\[ + \text{(contribution of all other triangles which do not involve the particle 0)} \]

\[
V_{u_1} (\begin{smallmatrix} y \\ x \\ 0 \end{smallmatrix}) = -\frac{\mu_1}{3a^2} \left\{ \begin{array}{l}
\left[ j \cdot (\hat{n}_3 - \frac{1}{3} \hat{n}_1) \right] \left[ i \cdot (\hat{n}_3 + \hat{n}_1) \right] \\
+ \left[ j \cdot (\hat{n}_5 - \frac{1}{3} \hat{n}_1) \right] \left[ i \cdot (\hat{n}_5 + \hat{n}_1) \right] \\
+ \left[ j \cdot (\hat{n}_7 - \frac{1}{3} \hat{n}_1) \right] \left[ i \cdot (\hat{n}_7 + \hat{n}_1) \right] \\
+ \left[ j \cdot (\hat{n}_9 - 2 \hat{n}_1) \right] \left[ i \cdot (\hat{n}_9 - \frac{2}{3} \hat{n}_1) \right] \\
+ \left[ j \cdot (\hat{n}_{11} - 2 \hat{n}_1) \right] \left[ i \cdot (\hat{n}_{11} - \frac{2}{3} \hat{n}_1) \right] \\
+ \left[ j \cdot (\hat{n}_{13} - 2 \hat{n}_1) \right] \left[ i \cdot (\hat{n}_{13} - \frac{2}{3} \hat{n}_1) \right] \end{array} \right\} = \frac{8\mu_1}{9a^2}
\]

From (2.16),

\[
V_{u_1} (\begin{smallmatrix} y \\ x \\ 0 \end{smallmatrix}) = \frac{8\mu_1}{9a^2}
\]

Similarly,
\[
\nu_{n_0} (\gamma x) = \begin{cases} 
\frac{8u_1}{9a^2} & (n=3, 4) \\
-\frac{8u_1}{9a^2} & (n=5, 6, 7, 8)
\end{cases}
\]  

(4.27)

\[
\nu_{1} (\gamma z) = -\frac{u_1}{6a^2} \left\{ [\hat{J} (\hat{N}_9 + 2\hat{N}_1)] [\hat{I} (\hat{N}_9 - \frac{2}{3} \hat{N}_3)] \\
+ [\hat{J} (\hat{N}_9 + 2\hat{N}_3)] [\hat{I} (\hat{N}_9 - \frac{2}{3} \hat{N}_5)] \\
+ [\hat{J} (\hat{N}_9 + 2\hat{N}_5)] [\hat{I} (\hat{N}_9 - \frac{2}{3} \hat{N}_8)] \\
+ [\hat{J} (\hat{N}_9 + 2\hat{N}_8)] [\hat{I} (\hat{N}_9 - \frac{2}{3} \hat{N}_6)] \right\} 
\]

(4.29)

\[
= 0
\]  

(4.30)

\[
\nu_{n_0} (\gamma x) = 0 \quad (n=10, 11, ..., 14)
\]  

(4.31)

From (2.18)

\[
\nu_{1} (\gamma z) = 0
\]  

(4.32)

By making use of equation (2.8), (4.25), (4.26), (4.27), (4.28), (4.30), (4.31) and (4.32), we have,
\[ \sum_{n} v_{\mu 1}^{x \ y} e^{i \hat{p} \cdot \hat{N}}_{n} = - \frac{64 \mu_1}{9a^2} s_1 s_2 c_3 \]  \hspace{1cm} (4.33) 

where \( s_1 \), and \( c_1 \) are defined in (3.19). Similarly, and making use of equations (2.18) and (2.8), we have

\[ v_{\mu 1}^{x \ y} = \begin{cases} 
- \frac{16 \mu_1}{9a^2} & \text{(n=1, 2, ..., 8)} \\
- \frac{32 \mu_1}{9a^2} & \text{(n=9, 10)} \\
\frac{8 \mu_1}{9a^2} & \text{(n=11, 12, 13, 14)} \\
\frac{160 \mu_1}{9a^2} & \text{(n=0)} 
\end{cases} \]  \hspace{1cm} (4.34) 

\[ \sum_{n} v_{\mu 1}^{x \ y} e^{i \hat{p} \cdot \hat{N}}_{n} = - \frac{128 \mu_1}{9a^2} c_1 c_2 c_3 - \frac{16 \mu_1}{9a^2} (4 \cos 2\pi a k_1 - \cos 2\pi a k_2 - \cos 2\pi a k_3) \]  \hspace{1cm} (4.36) 

\[ + \frac{160 \mu_1}{9a^2} \]  \hspace{1cm} (4.37)
where \( C_1 \) and \( S_i \) are defined in (3.19).

(11) Potential energy corresponding to \( u_2 \),

\[
V_{u_2} = \frac{1}{2} u_2 \left[ \left( \frac{s_1 - s_3}{a} \right) \cdot \hat{n}_{1,3,0} + \frac{(s_1 - s_0) \cdot \hat{n}_{1,0,3}}{\sqrt{3}a} \right]^2 \\
+ \left[ \frac{(s_3 - s_1) \cdot \hat{n}_{3,1,0}}{a} + \frac{(s_3 - s_0) \cdot \hat{n}_{3,0,1}}{\sqrt{3}a} \right]^2 \]

(This is the contribution of the type (1) triangle \( 0, 1, 3 \))

+ ... (contribution of the twelve type (1) triangles referring to the particle 0).

\[
+ \left( \frac{s_0 - s_9}{a} \right) \cdot \hat{n}_{0,9,1} + \frac{(s_0 - s_1) \cdot \hat{n}_{0,1,9}}{\sqrt{3}a} \]

\[
+ \left( \frac{s_9 - s_0}{a} \right) \cdot \hat{n}_{9,0,1} + \frac{(s_9 - s_1) \cdot \hat{n}_{9,1,0}}{\sqrt{3}a} \right]^2 \]

(This is the contribution of the type (2) triangle \( 0, 1, 9 \))

+ ... (contribution of the twenty-four type (2) triangles referring to the particle 0)

+ (contribution of all other triangles which do not involve the particle 0).

(4.39)

Making use of equations (4.16) to (4.20), (2.16), (2.18) and (2.8),

we have
\[
V_{\mu_2}(x, y) = \begin{cases} 
- \frac{4u_2}{3a^2} & (n=1, 2, 3, 4) \\
\frac{4u_2}{3a^2} & (n=5, 6, 7, 8) \\
0 & (n=9, 10, \ldots, 14) \\
0 & (n=0) 
\end{cases} 
\]

\[
\sum_n V_{\mu_2}(x, y) e^{i\vec{p} \cdot \vec{N}_n} = \frac{32u_2}{3a^2} s_1 s_2 s_3 
\]

\[
V_{\mu_2}(x, y) = \begin{cases} 
8\frac{u_2}{3a^2} & (n=1, 2, \ldots, 8) \\
- \frac{4u_2}{3a^2} & (n=11, 12, 13, 14) \\
80\frac{u_2}{3a^2} & (n=0) 
\end{cases} 
\]

\[
\sum_n V_{\mu_2}(x, y) e^{i\vec{p} \cdot \vec{N}_n} 
\]
\[
= \frac{80\mu_2}{3a^2} - \frac{64\mu_2}{3a^2} C_1C_2C_3 \\
- \frac{8\mu_2}{3a^2} (\cos 2\pi\alpha k_2 + \cos 2\pi\alpha k_3) \tag{4.49}
\]

where \(C_1\) and \(S_1\) are defined in (3.19)

Combination of \(\alpha_1, \alpha_2, \mu_1\) and \(\mu_2\) -

By combining equations (3.2), (4.9), (4.14), (4.33), (4.38), (4.44) and (4.49), we have a secular equation

\[
\begin{vmatrix}
P_1 - 4\pi^2 v^2 M & Q_{12} & Q_{13} \\
Q_{21} & P_2 - 4\pi^2 v^2 M & Q_{23} \\
Q_{31} & Q_{32} & P_3 - 4\pi^2 v^2 M
\end{vmatrix} = 0 \tag{4.50}
\]

where

\[
P_1 = \left\{ \frac{8\alpha_1}{3} + \frac{128\mu_1}{9a^2} + \frac{64\mu_2}{3a^2} (1 - C_1C_2C_3) + 4\alpha_2 S_1^2 - \frac{16\mu_1}{9a^2} \right\} \\
\times \left(4 \cos 2\pi\alpha k_1 - \cos 2\pi\alpha k_2 - \cos 2\pi\alpha k_3 - 2\right)
\]

\[
- \frac{8\mu_2}{3a^2} (\cos 2\pi\alpha k_2 + \cos 2\pi\alpha k_3 - 2) \right\}
\]

\[
Q_{12} = 8\left( \frac{\alpha_1}{3} - \frac{8\mu_1}{9a^2} + \frac{4\mu_2}{3a^2} S_1S_2C_3 \right)
\]
and the others can be obtained by circular permutations of the indices.

This is the same as that obtained by Clark et al. [23] equation (7) from first principles. The equivalence between the notations $\alpha, \beta, \gamma_1$ and $\gamma_2$ used in their paper and those we use, are shown in the following:

$$
\begin{align*}
\alpha &= \frac{a_1}{3} \\
\beta &= \alpha_2 \\
\gamma_1 &= \frac{8\mu_1}{9a^2} \\
\gamma_2 &= \frac{8\mu_2}{9a^2}
\end{align*}
$$

(4.52)

In the long-wave limit as $k \to 0$, with $\rho = 2M/a^3$, the secular equation obtained should be identical with the elasticity secular equation (3.22). Therefore, by comparison, we have

$$
2\alpha_2 + \frac{80\mu_1}{9a^2} - \frac{8\mu_2}{3a^2} = a c_{11} - a c_{44} \tag{4.53}
$$

$$
\frac{2\alpha_1}{3} + \frac{16\mu_1}{9a^2} + \frac{24\mu_2}{3a^2} = a c_{44} \tag{4.54}
$$

$$
\frac{4\alpha_1}{3} - \frac{32\mu_1}{9a^2} + \frac{16\mu_2}{3a^2} = a c_{12} + a c_{44} \tag{4.55}
$$
In the [100] direction, the phonon frequency at the first Brillouin zone boundary (i.e. \( k_1 = 1/a \)) is given by

\[
\nu_b = \frac{1}{\pi} \left[ \frac{1}{3M} (4\alpha_1 + \frac{64\mu_1}{3a^2} + \frac{32\mu_2}{a^2}) \right]^{1/2}
\]  

(4.56)

Solving equations (4.53) to (4.56), we have

\[
\alpha_1 = \frac{3}{4} a (e_{12} - e_{44}) + \frac{3}{4} \pi \nu_b^2 M \]

(4.57)

\[
\alpha_2 = \frac{1}{4} a (2e_{11} + e_{12} + 3e_{44}) - \frac{3}{4} \pi \nu_b^2 M
\]

(4.58)

\[
\frac{\mu_1}{a^2} = -\frac{9}{128} a (e_{12} + 3e_{44}) + \frac{9}{64} \pi \nu_b^2 M
\]

(4.59)

\[
\frac{\mu_2}{a^2} = -\frac{3}{64} a (e_{12} - 5e_{44}) - \frac{3}{32} \pi \nu_b^2 M
\]

(4.60)

By substituting (4.57), (4.58), (4.59) and (4.60) into (4.50), we have a secular equation

\[
\begin{bmatrix}
P_1 - 4\pi^2 \nu_b^2 M & Q_{12} & Q_{13} \\
Q_{21} & P_2 - 4\pi^2 \nu_b^2 M & Q_{23} \\
Q_{31} & Q_{32} & P_3 - 4\pi^2 \nu_b^2 M
\end{bmatrix} = 0
\]  

(4.61)
where

\[ P_1 = 2\pi^2 v_b^2 M \left( 1 - c_1 c_2 c_3 \right) + \left( 2a c_{11} - \pi v_b^2 M \right) S_1^2 + \left( 2a c_{44} - \pi v_b^2 M \right) (S_2^2 + S_3^2) \]

\[ Q_{12} = 2a (c_{12} + c_{44}) S_1 S_2 S_3 \]

and the remainder can be obtained by circular permutations of the indices. This is identical with that obtained in the angular force model I, namely equation (3.31). Hence the two angular force models (b.c.c.) are equivalent as far as the frequency spectrum is concerned.

(2) **Face-centered Cubic Lattice**

(See Fig. 4-3)

Since we only need to use terms of \( \left( \frac{\partial^2 v}{\partial u_0 \partial v_{n_0}} \right) \), we can treat the potential energy due to the central force interaction and the angular force interaction separately.

(a) **Central force (a1, a2) interaction** –

These are the same as those used in angular force model I (f.c.c. lattice). Therefore, the notations and results in that case are used here, namely, equations (3.38) and (3.44).

(b) **Angular force (κ1, κ2) interaction** –

There are two types of triangles which we are going to consider.
Fig. 4-3. The first and second neighbours of the particle 0 of the f.c.c. lattice.
The first one is that formed by a particle and two of its first neighbours which are both in the same plane of the coordinate axes. They are triangles equivalent to \(0, 1, 3\) in Fig. 4-3; particles 1 and 3 are both in the \(X-O-Z\) plane. This type of triangles is called type (1) triangles.

Since we intend to have closer comparison between the two angular force models when applied to both b.c.c. and f.c.c. lattices, we shall limit ourselves to models each consisting of two central force constants and two angular force constants.

The other type is that formed by a particle, one of its first neighbours and one of its second neighbours. They are triangles equivalent to \(\Delta 0, 1, 13\); particle 13 is a first neighbour of particle 1. This type of triangles is called type (2) triangles.

There are, in all, twelve type (1) triangles and twenty-four type (2) triangles, with reference to the particle 0. As shown in Fig. 4-3, all the thirty-six triangles are identical and each is isosceles with two equal angles \(\theta_2; \theta_2 = 45^\circ\). We shall associate with each angle \(\theta_1 (\theta_1 = 90^\circ)\) in the triangles an angular force constant \(\kappa_1\), and each angle \(\theta_2\) an angular force constant \(\kappa_2\).

The unit normals \(\hat{n}_{A,B,C}\) in (4.1) are given by

\[
\hat{n}_{1,0,j} = \frac{1}{\sqrt{2}} \hat{n}_j = \hat{n}_{0,1,j} \tag{4.62}
\]

\[
\hat{n}_{i,1,0} = -\frac{1}{2} (\hat{n}_i + \hat{n}_j) = \hat{n}_{j,1,0} \tag{4.63}
\]
\[ \hat{n}_{i,m,0} = -\frac{1}{\sqrt{2}} \hat{n}_i = \hat{n}_{m,i,0} \quad (4.64) \]

\[ \hat{n}_{0,i,m} = \frac{1}{\sqrt{2}} \hat{n}_j = \hat{n}_{i,0,m} \quad (4.65) \]

where \( \hat{N}_i + \hat{N}_j = \hat{N}_m \)

\[ \hat{n}_{m,0,i} = \hat{N}_1 - \frac{1}{2} \hat{N}_m = \hat{n}_{0,m,i} \quad (4.66) \]

where \( i, j \) denote the first neighbours of particle 0, and \( m \) the second neighbours.

We shall deal with the potential energy involving \( \kappa_1 \) first, then that involving \( \kappa_2 \).

(1) Potential energy involving \( \kappa_1 \),

\[ V_{\kappa_1} = \frac{1}{2} \kappa_1 \left\{ \frac{(s_0 - s_1) \cdot \hat{n}_{0,1,3}}{a/\sqrt{2}} + \frac{(s_0 - s_3) \cdot \hat{n}_{0,3,1}}{a/\sqrt{2}} \right\}^2 \]

(This is the contribution of the type (1) triangle \( 0,1,3 \))

+ ... (contribution of the twelve type (1) triangles referring to the particle 0)

\[ + \frac{(s_1 - s_0) \cdot \hat{n}_{1,0,13}}{a/\sqrt{2}} + \frac{(s_1 - s_3) \cdot \hat{n}_{1,13,0}}{a/\sqrt{2}} \]
(This is the contribution of the type (2) triangle 0, 1, 13) + ... (contribution of the twenty-four type (2) triangles referring to the particle 0) + (contribution of all other triangles which do not involve the particle 0) (4.67)

Making use of equations (4.62) to (4.66), (2.16), (2.18) and (2.8), we have

\[
V_{\kappa_1} (\vec{y} \vec{x} \mid \vec{n} \vec{0}) = \begin{cases} 
0 & \text{(n=1, 2, 3, 4)} \\
\frac{4\kappa_1}{a^2} & \text{(n=5, 6)} \\
-\frac{4\kappa_1}{a^2} & \text{(n=7, 8)} \\
0 & \text{(n=9, 10, 11, 12)} \\
0 & \text{(n=13, 14, ..., 18)} \\
0 & \text{(n=0)} 
\end{cases} \]

(4.68) (4.69) (4.70) (4.71) (4.72) (4.73)

\[
\sum_n V_{\kappa_1} (\vec{x} \vec{y} \mid \vec{n} \vec{0}) e^{i\vec{p} \cdot \vec{N}_n} = -\frac{16\kappa_1}{a^2} S_1 S_2 
\]

(4.74)
\[ V_{\kappa_1}^{(x,x)}_{n,0} = \begin{cases} 
\frac{-4\kappa_1}{a^2} & (n=1, 2, \ldots, 8) \\
0 & (n=9, 10, 11, 12) \\
\frac{-4\kappa_1}{a^2} & (n=13, 14) \\
\frac{2\kappa_1}{a^2} & (n=15, 16, 17, 18) \\
\frac{32\kappa_1}{a^2} & (n=0) 
\end{cases} \]  

(4.75)

(4.76)

(4.77)

(4.78)

(4.79)

\[ \sum_{n} V_{\kappa_1}^{(x,x)}_{n,0} \exp^{\mp i \cdot \mathbf{N}_n} \]

\[= \frac{32\kappa_1}{a^2} - \frac{16\kappa_1}{a^2} C_1(C_2 + C_3) - \frac{4\kappa_1}{a^2} \left(2 \cos 2\pi \kappa_1 - \cos 2\pi \kappa_2 - \cos 2\pi \kappa_3\right) \]

(4.80)

(ii) Potential energy involving $\kappa_2,$

\[ V_{\kappa_2} = \frac{1}{2} \kappa_2 \left\{ \begin{array}{l}
\left[ \frac{(\hat{s}_1 - \hat{s}_3) \cdot \hat{n}_{1,3,0}}{a} \right]^2 + \left[ \frac{(\hat{s}_1 - \hat{s}_2) \cdot \hat{n}_{1,1,0}}{a} \right]^2 + \left[ \frac{(\hat{s}_3 - \hat{s}_2) \cdot \hat{n}_{0,1,3}}{a} \right]^2 \\
+ \left[ \frac{(\hat{s}_3 - \hat{s}_1) \cdot \hat{n}_{3,1,0}}{a} \right]^2 + \left[ \frac{(\hat{s}_3 - \hat{s}_0) \cdot \hat{n}_{3,0,1}}{a} \right]^2 \end{array} \right. \]

(This is the contribution of the type (1) triangle 0,1,3)

+ ... (contribution of the twelve type (1) triangles referring to the particle 0).
\[ + \left[ \frac{\vec{s}_{0} \cdot \vec{s}_{13}}{a} \right] \cdot \vec{n}_{0,13,1} + \frac{\vec{s}_{0} \cdot \vec{s}_{1}}{a/\sqrt{2}} \cdot \vec{n}_{0,1,13} \left[ \frac{\vec{s}_{13} \cdot \vec{s}_{0}}{a} \right] \cdot \vec{n}_{13,0,1} + \frac{\vec{s}_{13} \cdot \vec{s}_{1}}{a/\sqrt{2}} \cdot \vec{n}_{13,1,0} \right] \]

(This is the contribution of the type (2) triangle 0,1,13).

\[ + \ldots \text{(contribution of the twenty-four type} \]

(2) triangles referring to the particle 0).

\[ + \text{(contribution of all other triangles which do not involve the particle 0)} \]

Making use of equations (4.62) to (4.66), (2.16), (2.18) and (2.8), we have

\[ \text{for} \ n = 0, 1, 2, \ldots, 18 \]

\[ V_{\kappa_{2}} \left( \begin{array}{c} x \\ y \\\end{array} \right) \left( \begin{array}{c} n \\ 0 \end{array} \right) = \begin{cases} 0 & (n=1, 2, \ldots, 12) \\ 0 & (n=13, 14, \ldots, 18) \\ 0 & (n=0) \end{cases} \] \hspace{2cm} (4.82)

\[ \sum_{n} V_{\kappa_{2}} \left( \begin{array}{c} x \\ y \\\end{array} \right) \left( \begin{array}{c} n \\ 0 \end{array} \right) e^{i \vec{p} \cdot \vec{n}} \left( \vec{n} \right) = 0 \] \hspace{2cm} (4.83)

\[ \sum_{n} = \begin{cases} \frac{4\kappa_{2}}{a^2} & (n=1, 2, \ldots, 8) \\ 0 & (n=9, 10, 11, 12) \\ 0 & (n=13, 14, \ldots, 18) \\ \frac{32\kappa_{2}}{a^2} & (n=0) \end{cases} \] \hspace{2cm} (4.84)

\[ V_{\kappa_{2}} \left( \begin{array}{c} x \\ y \\\end{array} \right) \left( \begin{array}{c} n \\ 0 \end{array} \right) = \begin{cases} 0 & (n=1, 2, \ldots, 8) \\ 0 & (n=9, 10, 11, 12) \\ 0 & (n=13, 14, \ldots, 18) \\ \frac{32\kappa_{2}}{a^2} & (n=0) \end{cases} \] \hspace{2cm} (4.85)

\[ (4.86) \]

\[ (4.87) \]

\[ (4.88) \]

\[ (4.89) \]
\[
\sum_{n} V_{k_2} \left( x_n \right) e^{i \mathbf{p} \cdot \mathbf{n}}
= \frac{32 \kappa_2}{a^2} - \frac{16 \kappa_2}{a^2} \ C_1 (C_2 + C_3)
\]
(4.90)

Combination of \( \alpha_1, \alpha_2, \kappa_1, \kappa_2 \) -

By combining equations (3.2), (3.38), (3.44), (4.74), (4.80), (4.85) and (4.90), we have a secular equation

\[
\begin{vmatrix}
R_1 - 4 \pi^2 \nu^2 M & T_{12} & T_{13} \\
T_{21} & R_2 - 4 \pi^2 \nu^2 M & T_{23} \\
T_{31} & T_{32} & R_3 - 4 \pi^2 \nu^2 M
\end{vmatrix} = 0
\]
(4.91)

Where
\[
R_1 = 2\left[ \alpha_1 + \frac{8}{a^2} (\kappa_1 + \kappa_2) \right] [2 - C_1 (C_2 + C_3)] + 4 \alpha_2 S_1^2 - \frac{4 \kappa_1}{a^2} \ x
\]
\[
x(2 \cos 2 \pi \alpha_1 - 2 \kappa_1 - 2 \cos 2 \pi \kappa_2)
\]

\[
T_{12} = \left( 2 \alpha_1 - \frac{16 \kappa_1}{a^2} \right) S_1 S_2
\]

and the others can be obtained by circular permutations of the indices.

\( C_1, S_1 \) are defined in (3.19)
In the long-wave limit as \( k \rightarrow 0 \), with \( \rho = 4M/a^3 \), the secular equation should be identical with the elasticity secular equation (3.22). Therefore, by comparison, we have

\[
\alpha_1 + \frac{8}{a^2} (4\kappa_1 + \kappa_2) + 4\alpha_2 = \alpha_{11} - \alpha_{44} \tag{4.92}
\]

\[
\alpha_1 + \frac{8}{a^2} \kappa_2 = \alpha_{44} \tag{4.93}
\]

\[
2\alpha_1 - \frac{16}{a^2} \kappa_1 = \alpha_{12} + \alpha_{44} \tag{4.94}
\]

(longitudinal)

The phonon frequency in the [100] direction at the Brillouin zone boundary (i.e. \( \kappa_1 = 1/a \)), is given by:

\[
\nu_b = \frac{1}{\pi} \left\{ \frac{2}{M} \left[ \alpha_1 + \frac{8}{a^2} (\kappa_1 + \kappa_2) \right] \right\}^{1/2} \tag{4.95}
\]

Solving equations (4.92) to (4.95), we have

\[
\alpha_1 = \frac{1}{2} a(c_{12} - c_{44}) + \frac{1}{2} \pi^2 \nu_b^2 M \tag{4.96}
\]

\[
\alpha_2 = \frac{1}{4} a(c_{11} + 2c_{44}) - \frac{1}{2} \pi^2 \nu_b^2 M \tag{4.97}
\]
\[ \frac{\kappa_1}{a^2} = -\frac{1}{8} ac_{44} + \frac{1}{16} \pi^2 v_b^2 M \] (4.98)

\[ \frac{\kappa_2}{a^2} = -\frac{1}{16} a(c_{12} - 3c_{44}) - \frac{1}{16} \pi^2 v_b^2 M \] (4.99)

By substituting (4.96), (4.97), (4.98) and (4.99) into (4.91), we have a secular equation

\[
\begin{vmatrix}
R_1 - 4\pi^2 v_b^2 M & T_{12} & T_{13} \\
T_{21} & R_2 - 4\pi^2 v_b^2 M & T_{23} \\
T_{31} & T_{32} & R_3 - 4\pi^2 v_b^2 M
\end{vmatrix} = 0
\] (4.100)

where

\[ R_1 = \pi^2 v_b^2 M \left[ 2 - c_1(c_2 + c_3) \right] + (ac_{11} - \pi^2 v_b^2 M) S_1^2 \]

\[ + (ac_{44} - \frac{1}{2} \pi^2 v_b^2 M) (S_2^2 + S_3^2) \]

\[ T_{12} = a(c_{12} + c_{44}) S_1 S_2 \]

and the others can be obtained by circular permutations of the indices.

Comparing (3.61) and (4.100), we find that

\[ K_i \neq R_i \] (4.101)

but

\[ L_{ij} = T_{ij} \] (4.102)
CHAPTER V

DATA AND CALCULATIONS

The frequency histograms are obtained following the method used by Varshni and Shukla [26] by means of a 1620 IBM computer. The first Brillouin zone is divided into identical cubes each of edge equal to 1/40 of the distance between \( \Gamma \) and \( X \) points of the Brillouin zone. The total number of such cubes in the first zone is 64000, and that of frequencies is 192000. Because of symmetric properties, we need only consider 1/48 of the first zone. This has 1686 points; each point is weighed according to the number of points equivalent to it. Special attention has to be paid to those points lying on the surfaces, edges and corners of the first zone. The frequencies are obtained by solving the appropriate secular equations. The frequency histograms are then obtained by Blackman's sampling method.

For all the metals which we deal with, except nickel and sodium, the histograms are obtained from data at 0°K and the dispersions curves from data at temperatures at which the experimental dispersion curves are obtained. For the cases of nickel and sodium, the histograms are obtained at temperatures other than 0°K because no elastic constant data at 0°K are available.

Because experimental values of phonon frequency (longitudinal) at the first zone boundary in the [100] direction at 0°K, \( v_D(0) \) are not
available, we obtain these values by means of the following method.

It is well known that for longitudinal elasticity waves in the [100] direction (see, e.g., de Launay's article [12], equation (10.10)),

\[ v_{k(\text{elast.})} (t) = \left[ \frac{c_{ll} (t)}{\rho (t)} \right]^{1/2} \] (5.1)

where \( v_{k(\text{elast.})} (t) \) is the frequency of the elasticity wave (longitudinal) in the [100] direction and at \( t^\circ K \). With \( \rho (t) = \frac{2M}{a^3 (t)} \) for b.c.c. lattice or \( \rho (t) = \frac{4M}{a^3 (t)} \) for f.c.c. lattice, we have

\[ \frac{v_{k(\text{elast.})} (0)}{v_{k(\text{elast.})} (t)} = \left[ \frac{c_{ll} (0) a^3 (0)}{c_{ll} (t) a^3 (t)} \right]^{1/2} \] (5.2)

We assume that this relation is true for all values of \( k \),

i.e.,

\[ \frac{v_k (0)}{v_k (t)} = \left[ \frac{c_{ll} (0) a^3 (0)}{c_{ll} (t) a^3 (t)} \right]^{1/2} \] (5.3)

for all \( k \).
In particular, we have

\[
\frac{v_b(0)}{v_b(t)} = \left[ \frac{c_{11}(0) a^3(0)}{c_{11}(t) a^3(t)} \right]^{1/2}
\]  

(5.4)

where \(v_b(t)\) is the boundary phonon frequency (longitudinal) in the [100] direction and at \(t^\circ K\).

The lattice specific heats at constant volume are then calculated from the expression,

\[
C_v = 3R \int_0^{\nu_m} \frac{x^2 e^x}{(e^x - 1)^2} g(v) \, dv
\]

(5.5)

where \(x = \frac{\hbar v}{kT}\)

and

\[
\int_0^{\nu_m} g(v) \, dv = 1
\]

The equivalent Debye temperatures are then calculated from the relation

\[
\frac{C_v}{3R} = \frac{4\pi^4}{5} \left( \frac{T}{\theta} \right)^3 - \frac{3\theta/T}{e^{\theta/T} - 1} + 12 \log (1-e^{-\theta/T}) = 36 \frac{T}{\theta} \sum_{n=1}^{\infty} \left\{ \frac{n+2T}{n\theta} + \frac{2}{n^2} \left( \frac{T}{\theta} \right)^2 \right\} 
\]

\[
x \frac{e^{-n\theta/T}}{n^2}
\]

(5.6)
(1) **Face-centered Cubic Lattice**

The metals which we deal with are copper, aluminum and nickel. The lattice constant \((a)\), elastic constants \((c_{11}, c_{12}, c_{44})\) and the phonon frequency (longitudinal) at the zone boundary in the [100] direction \((\nu_b)\) of these metals are shown in Table 2.
Table 2. The lattice constant (a), the elastic constants (c_{11}, c_{12}, c_{44}) and the phonon frequency (longitudinal) at the zone boundary in the [100] direction, (v_{b}) of copper, aluminum and nickel.

<table>
<thead>
<tr>
<th>Group</th>
<th>Element</th>
<th>Temp.</th>
<th>a</th>
<th>C_{11}</th>
<th>C_{12}</th>
<th>C_{44}</th>
<th>Ref.</th>
<th>Temp.</th>
<th>[100]v_{b}</th>
</tr>
</thead>
<tbody>
<tr>
<td>1b</td>
<td>Cu</td>
<td>0</td>
<td>3.6029</td>
<td>17.62</td>
<td>12.494</td>
<td>8.177</td>
<td>c</td>
<td>0</td>
<td>7.43</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>3.6147</td>
<td>16.839</td>
<td>12.142</td>
<td>7.539</td>
<td>c</td>
<td>300</td>
<td>7.3</td>
</tr>
<tr>
<td>3b</td>
<td>Al</td>
<td>0</td>
<td>4.0328</td>
<td>11.430</td>
<td>6.192</td>
<td>3.162</td>
<td>d</td>
<td>0</td>
<td>9.73</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80</td>
<td>4.0338</td>
<td>11.373</td>
<td>6.191</td>
<td>3.128</td>
<td>d</td>
<td>80</td>
<td>9.71</td>
</tr>
<tr>
<td>8</td>
<td>Ni</td>
<td>296</td>
<td>3.5236</td>
<td>24.6</td>
<td>15.0</td>
<td>12.2</td>
<td>e</td>
<td>296</td>
<td>8.55</td>
</tr>
</tbody>
</table>

a Calculated from the room temperature value by the method of Corruccini and Galewew [29].
b A.I.P. Handbook [30].
c Overton and Caffney [31].
d Kamm and Alers [32].
e de Klerk [33].
f Derived from the experimental value at higher temperature as explained in the text (equation (5.4)).
g Sinha [34] and Svensson, Brockhouse and Rowe [35].
h Stedman and Nilsson [36].
i Birgeneau et al. [37].
(I) Angular force model I -

The values of the interparticle force constants $\alpha_1$, $\alpha_2$, $\sigma_1$ and $\sigma_2$ are obtained from equations (3.57), (3.58), (3.59) and (3.60). These are shown in Table 3.

Table 3. The interparticle force constants $\alpha_1$, $\alpha_2$, $\sigma_1$ and $\sigma_2$ of copper, aluminum and nickel in the angular force model I.

<table>
<thead>
<tr>
<th>Group</th>
<th>Metal</th>
<th>Temp. (°K)</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\sigma_1$ ($10^3$ dynes/cm.)</th>
<th>$\sigma_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1b</td>
<td>Cu</td>
<td>0</td>
<td>32.99</td>
<td>1.500</td>
<td>-4.248</td>
<td>2.304</td>
</tr>
<tr>
<td>3b</td>
<td>Al</td>
<td>0</td>
<td>19.90</td>
<td>1.058</td>
<td>1.035</td>
<td>-2.562</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>31.66</td>
<td>1.344</td>
<td>-3.913</td>
<td>1.833</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80</td>
<td>19.82</td>
<td>1.047</td>
<td>1.025</td>
<td>-2.569</td>
</tr>
<tr>
<td>8</td>
<td>Ni</td>
<td>296</td>
<td>41.54</td>
<td>4.087</td>
<td>-6.377</td>
<td>5.144</td>
</tr>
</tbody>
</table>

The theoretical dispersion curves are obtained from equation (3.52) and are shown in Fig. 6-1 (copper), Fig. 6-6 (aluminum) and Fig. 6-11 (nickel) along with the experimental points.

The frequency histograms are shown in Fig. 6-3 (copper), Fig. 6-8 (aluminum) and Fig. 6-13 (nickel).

The equivalent Debye temperatures obtained from equation (5.6)
are shown in Fig. 6-5 (copper), Fig. 6-10 (aluminum) and Fig. 6-15 (nickel) together with the experimental values.

(II) Angular force model II -

The values of the interparticle force parameters $\alpha_1$, $\alpha_2$, $\kappa_1/(a^2)$ and $\kappa_2/(a^2)$ are obtained from equations (4.96), (4.97), (4.98) and (4.99).

These are shown in Table 4.

Table 4. The interparticle force parameters $\alpha_1$, $\alpha_2$, $\kappa_1/(a^2)$ and $\kappa_2/(a^2)$ of copper, aluminum and nickel in angular force model II.

<table>
<thead>
<tr>
<th>Group</th>
<th>Metal</th>
<th>Temp. (°K)</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\kappa_1/(a^2)$</th>
<th>$\kappa_2/(a^2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1b</td>
<td>Cu</td>
<td>0</td>
<td>36.52</td>
<td>1.859</td>
<td>-0.090</td>
<td>-0.882</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>36.06</td>
<td>1.098</td>
<td>0.0617</td>
<td>-1.102</td>
</tr>
<tr>
<td>3b</td>
<td>Al</td>
<td>0</td>
<td>27.04</td>
<td>-3.031</td>
<td>1.022</td>
<td>-1.786</td>
</tr>
<tr>
<td></td>
<td></td>
<td>80</td>
<td>27.02</td>
<td>-3.067</td>
<td>1.028</td>
<td>-1.801</td>
</tr>
<tr>
<td>8</td>
<td>Ni</td>
<td>296</td>
<td>40.10</td>
<td>7.997</td>
<td>-0.9776</td>
<td>0.3610</td>
</tr>
</tbody>
</table>

The dispersion curves obtained from equation (4.91) are shown in Fig. 6-2 (copper), Fig. 6-7 (aluminum) and Fig. 6-12 (nickel).

The frequency histograms are shown in Fig. 6-4 (copper),
Fig. 6-9 (aluminum) and Fig. 6-14 (nickel), and the equivalent Debye temperatures obtained from equation (5.6) are shown in Fig. 6-5 (copper), Fig. 6-10 (aluminum) and Fig. 6-15 (nickel).

(2) **Body-centered Cubic Lattice**

The following metals have been considered: sodium, tantalum, molybdenum, tungsten, and iron. The lattice constant \( a \), the elastic constants \( c_{11}, c_{12}, c_{44} \) and the phonon frequency (longitudinal) at the zone boundary in the [100] direction \( \nu_b \) of these metals are shown in Table 5.
Table 5. The lattice constant (a), the elastic constants \( (c_{11}, c_{12}, c_{44}) \) and the phonon frequency (longitudinal) at the zone boundary in the [100] direction \( (\nu_L) \) of sodium, tantalum, Molybdenum, tungsten and iron.

<table>
<thead>
<tr>
<th>Group</th>
<th>Element</th>
<th>Temp. ( (^\circ K) )</th>
<th>a ( (10^{-8} \text{ cm.}) )</th>
<th>( C_{11} ) ( (10^{11} \text{ dyn/cm}^2) )</th>
<th>( C_{12} ) ( (10^{11} \text{ dyn/cm}^2) )</th>
<th>( C_{44} ) ( (10^{11} \text{ dyn/cm}^2) )</th>
<th>Ref.</th>
<th>Temp. ( (^\circ K) )</th>
<th>[100] ( \nu_L ) ( (10^{12} \text{ cps}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>la</td>
<td>Na</td>
<td>78</td>
<td>4.2353(^a)</td>
<td>0.815</td>
<td>0.679</td>
<td>0.578</td>
<td>c</td>
<td>90</td>
<td>3.58(^g)</td>
</tr>
<tr>
<td>5a</td>
<td>Ta</td>
<td>0</td>
<td>3.2979(^a)</td>
<td>26.632</td>
<td>15.816</td>
<td>8.736</td>
<td>{}</td>
<td>0</td>
<td>5.07(^h)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>3.3026(^b)</td>
<td>26.091</td>
<td>15.743</td>
<td>8.182</td>
<td>d</td>
<td>296</td>
<td>5.03(^i)</td>
</tr>
<tr>
<td></td>
<td>Mo</td>
<td>0</td>
<td>3.1470(^a)</td>
<td>45.002</td>
<td>17.292</td>
<td>12.503</td>
<td>{}</td>
<td>0</td>
<td>6.357(^j)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>3.1500(^b)</td>
<td>44.077</td>
<td>17.243</td>
<td>12.165</td>
<td>d</td>
<td>296</td>
<td>6.3(^k)</td>
</tr>
<tr>
<td>6a</td>
<td>W</td>
<td>0</td>
<td>3.1620(^a)</td>
<td>53.255</td>
<td>20.495</td>
<td>16.313</td>
<td>{}</td>
<td>0</td>
<td>5.54(^h)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>3.1648(^b)</td>
<td>52.327</td>
<td>20.453</td>
<td>16.072</td>
<td>d</td>
<td>room</td>
<td>5.50(^l)</td>
</tr>
<tr>
<td>8</td>
<td>Fe</td>
<td>0</td>
<td>2.8608(^a)</td>
<td>24.31</td>
<td>13.81</td>
<td>12.19</td>
<td>e</td>
<td>0</td>
<td>8.433(^h)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>289</td>
<td>2.8665(^b)</td>
<td>23.35</td>
<td>13.55</td>
<td>11.8</td>
<td>e, f</td>
<td>289</td>
<td>8.29(^m)</td>
</tr>
</tbody>
</table>

\(^a\) Calculated from the room temperature value [30] by the method of Corruccini and Gniewek [29].

\(^b\) A.I.P. Handbook [30].

\(^c\) Diederich and Trivisonno [38].

\(^d\) Featherston and Neighbours [39].
Rayne and Chandrasekhar [40].

Low [41].

Woods et al. [42].

Derived from the experimental value at higher temperature as explained in the text (equation 5.4)).

Woods [43].

Derived from the room temperature value ($6.3 \times 10^{12}$ cps.) as explained in the text (equation (5.4))

Woods and Chen [44]. This is not the experimental value but rather the value given by the force constant model used by these authors. It was found that this value gives a better overall agreement with the dispersion curves.

Chen and Brockhouse [45].

Low [41].
(I) Angular force model I -

The values of the interparticle force constants $\alpha_1$, $\alpha_2$, $\eta_1$ and $\eta_2$ are obtained from equations (3.27), (3.28), (3.29) and (3.30). These are shown in Table 6.

Table 6. The interparticle force constants $\alpha_1$, $\alpha_2$, $\eta_1$ and $\eta_2$ of sodium, tantalum, molybdenum, tungsten and iron in angular force model I.

<table>
<thead>
<tr>
<th>Group</th>
<th>Metal</th>
<th>Temp. (°K)</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\eta_1$ (10$^3$ dynes/cm)</th>
<th>$\eta_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>Na</td>
<td>78</td>
<td>3.8690</td>
<td>0.5187</td>
<td>-0.1237</td>
<td>0.0168</td>
</tr>
<tr>
<td>5a</td>
<td>Ta</td>
<td>0</td>
<td>59.54</td>
<td>24.86</td>
<td>-1.187</td>
<td>-4.651</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>58.26</td>
<td>24.33</td>
<td>-0.997</td>
<td>-5.246</td>
</tr>
<tr>
<td></td>
<td>Mo</td>
<td>0</td>
<td>62.77</td>
<td>54.93</td>
<td>-7.557</td>
<td>3.789</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>61.92</td>
<td>53.82</td>
<td>-7.558</td>
<td>3.559</td>
</tr>
<tr>
<td>6a</td>
<td>W</td>
<td>0</td>
<td>81.31</td>
<td>61.08</td>
<td>-5.979</td>
<td>2.673</td>
</tr>
<tr>
<td></td>
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<td>80.58</td>
<td>60.02</td>
<td>-6.114</td>
<td>2.647</td>
</tr>
<tr>
<td>8</td>
<td>Fe</td>
<td>0</td>
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<td>18.50</td>
<td>-2.324</td>
<td>1.165</td>
</tr>
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<td></td>
<td></td>
<td>289</td>
<td>52.06</td>
<td>17.74</td>
<td>-2.442</td>
<td>1.188</td>
</tr>
</tbody>
</table>
(II) Angular force model II -

The values of the interparticle force parameters $\alpha_1$, $\alpha_2$, $\mu_1/(a^2)$ and $\mu_2/(a^2)$ are obtained from equations (4.57), (4.58), (4.59) and (4.60). These are shown in Table 7.

Table 7. The interparticle force parameters $\alpha_1$, $\alpha_2$, $\mu_1/(a^2)$ and $\mu_2/(a^2)$ of sodium, tantalum, molybdenum, tungsten and iron in angular force model II.

<table>
<thead>
<tr>
<th>Group</th>
<th>Metal</th>
<th>Temp.</th>
<th>$\alpha_1$</th>
<th>$\alpha_2$</th>
<th>$\mu_1/(a^2)$</th>
<th>$\mu_2/(a^2)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1a</td>
<td>Na</td>
<td>78</td>
<td>3.942</td>
<td>0.6593</td>
<td>-0.0395</td>
<td>0.0137</td>
</tr>
<tr>
<td>5a</td>
<td>Ta</td>
<td>0</td>
<td>74.68</td>
<td>21.39</td>
<td>0.974</td>
<td>-2.839</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>75.00</td>
<td>20.08</td>
<td>1.195</td>
<td>-3.138</td>
</tr>
<tr>
<td>6a</td>
<td>Mo</td>
<td>0</td>
<td>58.96</td>
<td>66.27</td>
<td>-3.191</td>
<td>0.715</td>
</tr>
<tr>
<td></td>
<td></td>
<td>300</td>
<td>58.80</td>
<td>64.94</td>
<td>-3.127</td>
<td>0.585</td>
</tr>
<tr>
<td>8</td>
<td>Fe</td>
<td>0</td>
<td>79.27</td>
<td>69.73</td>
<td>-2.433</td>
<td>0.383</td>
</tr>
<tr>
<td></td>
<td></td>
<td>289</td>
<td>50.94</td>
<td>21.37</td>
<td>-1.021</td>
<td>0.210</td>
</tr>
</tbody>
</table>

Because equations (3.31) and (4.61) are identical, the two
angular force models for the b.c.c. lattice are equivalent as far as the frequency spectrum is concerned. We can use any one of equations (3.20), (3.31) (i.e. (4.61)) and (4.50) for obtaining the dispersion curves, frequency histograms and hence the equivalent Debye temperatures.

We use equation (4.50) to obtain the dispersion curves. These are shown together with the experimental points in Fig. 6-16 (sodium), Fig. 6-19 (tantalum), Fig. 6-22 (molybdenum), Fig. 6-25 (tungsten) and Fig. 6-28 (iron).

The frequency histograms are obtained from equation (4.50) and are shown in Fig. 6-17 (sodium), Fig. 6-20 (tantalum), Fig. 6-23 (molybdenum), Fig. 6-26 (tungsten) and Fig. 6-29 (iron).

With the specific heats obtained from equation (5.5), the equivalent Debye temperatures are obtained from equation (5.6) and are shown in Fig. 6-18 (sodium), Fig. 6-21 (tantalum), Fig. 6-24 (molybdenum), Fig. 6-27 (tungsten) and Fig. 6-30 (iron) along with the experimental values.
CHAPTER VI

RESULTS, DISCUSSIONS AND CONCLUSION

As mentioned in Chapter I, the most general force constant model is the tensor-force model. In the following, we shall discuss the interpretation of the two angular force models (AFM-I and AFM-II) in terms of the tensor force model, and the results we obtained.

(1) Face-centered Cubic Lattice -

Upon equating secular equation (3.52) and the secular equation of a tensor-force model with first neighbour and second neighbour interactions for the f.c.c. lattice*, we find that, as far as the frequency spectrum is concerned, the angular force model I for f.c.c. lattice is equivalent to a particular case of the tensor-force model with

\[
\begin{align*}
\alpha_1^{110} &= \frac{1}{2} (\alpha_1 + \alpha_1) \\
\alpha_3^{110} &= 2\alpha_1
\end{align*}
\]  

(6.1)

(6.2)

* See, e.g., Squires' article [21], Table II. The second term in \( M_{11} \) for the f.c.c. lattice should read \( \left\{ \begin{array}{c}
110 \\
2\alpha_3 (1 - \cos \theta_2 \cos \theta_3)
\end{array} \right\}. \)
\[
\beta_3 = \frac{1}{2} (\alpha_1 - \sigma_1)
\] 
\[(6.3)\]

\[
\alpha_1 = \alpha_2
\] 
\[(6.4)\]

and

\[
\alpha_2 = \sigma_2
\] 
\[(6.5)\]

where \(\alpha_1, \alpha_3, \beta_3, \alpha_1, \) and \(\alpha_2\) are notation used by Squires [21] to denote the force parameters for the first and the second neighbours, used in the tensor-force model. From (6.1), (6.2) and (6.3), we have a relation between the first neighbour tensor-force parameters,

\[
2\alpha_1 - \alpha_3 - 2\beta_3 = 0
\] 
\[(6.6)\]

Upon equating secular equation (4.91) and the secular equation of a tensor-force model with first neighbour and second neighbour interactions for the f.c.c. lattice (see footnote in p. 74), we find that, as far as the frequency spectrum is concerned, the angular force model II for f.c.c. lattice is equivalent to a particular case of the tensor-force model with
\[ a_{110}^1 = \frac{1}{2} a_1 + \frac{4}{a^2} (\kappa_1 + \kappa_2) \]  
(6.7)

\[ a_{3}^{110} = 0 \]  
(6.8)

\[ b_{3}^{110} = \frac{1}{2} a_1 - \frac{4}{a^2} \kappa_1 \]  
(6.9)

\[ a_1^{200} = a_2 + \frac{4}{a^2} \kappa_1 \]  
(6.10)

\[ a_2^{200} = -\frac{2}{a^2} \kappa_1 \]  
(6.11)

Dispersion curves by the angular force model I for the face-centered cubic lattice —

From equation (3.61), we have obtained equations for the dispersion curves along some axes of symmetry.

(i) [100] direction.

Longitudinal lattice wave frequency,

\[ \nu(L) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ 2\pi^2 v_b^2 M(1-C_1) + (a c_{11} - \pi v_b^2 M S_1^2) \right] \right\}^{1/2} \]  
(6.12)
Transverse lattice wave frequency,

\[ v(T) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ (ac_{12} + ac_{44} - 2\pi v_b^2 M) (c_1-1) \right] \\
+ \left( \frac{1}{2} ac_{12} + \frac{3}{2} ac_{44} + \pi v_b^2 M \right) \right\}^{1/2} \] (6.13)

(ii) [110] direction.

Longitudinal lattice wave frequency,

\[ v(L) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ (ac_{12} + ac_{44} - 2\pi v_b^2 M) (c_1-1) \right] \\
+ \left( ac_{11} + \frac{3}{2} ac_{12} + \frac{5}{2} ac_{44} - \pi v_b^2 M \right) \right\}^{1/2} \] (6.14)

Transverse lattice waves' frequencies,

\[ v(T_1) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ (ac_{12} + ac_{44} - 2\pi v_b^2 M) (c_1-1) \right] \\
+ \left( ac_{11} - \frac{1}{2} ac_{12} + \frac{1}{2} ac_{44} - \pi v_b^2 M \right) \right\}^{1/2} \] (6.15)

and

\[ v(T_2) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ 2\pi v_b^2 M (1-c_1) + (2ac_{44} - \pi v_b^2 M) \right] \right\}^{1/2} \] (6.16)
(iii) [111] direction

Longitudinal lattice wave frequency,

\[ v(L) = \frac{1}{2\pi} \left\{ \frac{a}{M} \left[ c_{11} + 2c_{12} + 4c_{44} \right] \right\}^{1/2} S_1 \quad (6.17) \]

Transverse lattice wave frequency,

\[ v(T) = \frac{1}{2\pi} \left\{ \frac{a}{M} \left[ c_{11} - c_{12} + c_{44} \right] \right\}^{1/2} S_1 \quad (6.18) \]

Dispersion curves by the angular force model II for the face-centered cubic lattice -

From equation (4.100), we have obtained equations for the axes dispersion curves along some of symmetry.

(1) [100] direction.

Longitudinal lattice wave frequency,

\[ v(L) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ 2\pi^2 \nu_b^2 \left( 1-C_1 \right) + (ae_{11} - \frac{1}{2} \pi^2 \nu_b^2 M) S_1^2 \right] \right\}^{1/2} \quad (6.19) \]

Transverse lattice wave frequency

\[ v(T) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ \pi^2 \nu_b^2 \left( 1-C_1 \right) + (ae_{44} - \frac{1}{2} \pi^2 \nu_b^2 M) S_1^2 \right] \right\}^{1/2} \quad (6.20) \]
(11) [110] direction

Longitudinal lattice wave frequency,

\[ \nu(L) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ \pi^2 v_b^2 M (1-C_1) + (ac_{11} + ac_{12} + 2ac_{44} - \frac{1}{2} \pi^2 v_b^2 M) S_1^2 \right] \right\}^{1/2} \]

Transverse lattice waves' frequencies,

\[ \nu(T_1) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ \pi^2 v_b^2 M (1-C_1) + (ac_{11} - ac_{12} - \frac{1}{2} \pi^2 v_b^2 M) S_1^2 \right] \right\}^{1/2} \]  
(6.21)

\[ \nu(T_2) = \frac{1}{2\pi} \left\{ \frac{1}{M} \left[ 2\pi^2 v_b^2 M (1-C_1) + (2ac_{44} - \pi^2 v_b^2 M) S_1^2 \right] \right\}^{1/2} \]  
(6.22)

(iii) [111] direction

Longitudinal lattice wave frequency,

\[ \nu(L) = \frac{1}{2\pi} \left\{ \frac{a}{M} \left[ c_{11} + 2c_{12} + 4c_{44} \right] \right\}^{1/2} S_1 \]  
(6.24)

Transverse lattice wave frequency,

\[ \nu(T) = \frac{1}{2\pi} \left\{ \frac{a}{M} \left[ c_{11} - c_{12} + c_{44} \right] \right\}^{1/2} S_1 \]  
(6.25)

On comparing equations (6.12) and (6.19), (6.16) and (6.23), (6.17) and (6.24), (6.18) and (6.25), we find that the longitudinal dispersion curves in the [100] direction, the transverse dispersion curves
$T_2$ (vibrating along the [001] direction) in the [110] direction, the longitudinal and the transverse dispersion curves in the [111] direction, are identical for the two angular force models. This is also seen in the corresponding figures.

Upon examining Tables 3 and 4 in Chapter V, we find that for both models, in general, the first neighbour central force parameter, $\alpha_1$, is of magnitude ten to twenty times those of the corresponding second neighbour force parameter, $\alpha_2$. For the metals investigated, all $\alpha_1$ and $\alpha_2$ are positive except $\alpha_2$ of aluminum in Model II. In general, the angular force parameters in Model I, $\sigma_1$ and $\sigma_2$ are of the same order of magnitude as $\alpha_2$ while those in Model II are smaller. The angular force parameters/Model II are smaller in magnitude than those in Model I. Their signs vary from metal to metal and from model to model. In the case of copper, $\kappa_1/(a^2)$ is very small in comparison with the others.

Copper

On examining the dispersion curves of copper (Figs. 6-1 and 6-2), we find that in the [$\xi00$] and the [$\xi00$] direction, Model II gives reasonably good result while the transverse dispersion curve along the [$\xi00$] direction and the dispersion curve $T_2$ in the [$\xi00$] direction in Model I gives values below that of the experimental points by about 15%. The dispersion curves in the [$\xi\xi\xi$] direction are satisfactory. (They are identical for these two models). The experimental values shown in the
Fig. 6.1 (a) Copper (AFM - 1, 300°C)
Fig. 6-1(b) Copper (AFM-11, 300°K)
Fig. 6-2(a). Dispersion curves of copper by AFM-II at 300°K.
Fig. 6-2(b) Dispersion curves of copper by AFM-II at 300°K.
Cu
AFM-I

Fig. 6-3.
Fig. 6-4. Frequency Spectra of Copper.
diagrams are due to Sinha [34] and Cribier [46]. Very similar results have been obtained by Svensson, Brockhouse and Rowe [35] by a different method.

The frequency spectrum of copper in model I (Fig. 6-3) has a broad peak at frequency about $4 \times 10^{12}$ cps and a sharp peak of approximately the same height at a frequency of $7 \times 10^{12}$ cps. The frequency spectrum of copper in model II (Fig. 6-4) has a broad peak at about $4.5 \times 10^{12}$ cps and a sharp peak of about double its height at $7 \times 10^{12}$ cps. This spectrum is in good agreement with that obtained by Varshni and Shukla [26], using a third-neighbour tensor-force model.

The Debye temperature curves of copper for the two models are of the same shape (Fig. 6-5). Model II gives better agreement with the experimental results at low temperature while model I gives better results at higher temperature. Moreover, it approaches to a constant value of about $312^\circ K$ for temperatures higher than $140^\circ K$. The experimental values of Debye temperatures are from Martin [47, 48].

**Aluminum**

In the case of aluminum, Model II gives better result of dispersion curves than that of Model I (Figs. 6-6 and 6-7). The longitudinal dispersion curve in the $[\xi 00]$ direction, the transverse dispersion curve $T_2$ in the $[\xi \xi 0]$ direction and the transverse dispersion curve in the $[\xi \xi \xi]$ direction are reasonable. The experimental values have been obtained by Stedman and Nilsson [36] at $80^\circ K$. 
REDUCED WAVE VECTOR PARAMETER, $\xi = a k_i$

Fig. 6-6 Aluminum (AFM-1, 80\(^\circ\)K)
Fig. 6-7. Dispersion curves of Aluminum by AFM-II (80°C K).
Fig. 6-9. Frequency Spectra of Aluminum.
The frequency spectra of aluminum for the two models are similar (Figs. 6-8 and 6-9). Both give a broad peak in the range of ω from $5 \times 10^{12}$ cps to $7 \times 10^{12}$ cps, and a sharper and higher peak at about $8.8 \times 10^{12}$ cps. These are compatible with that obtained by Varshni and Shukla [26], using an axially symmetric model.

The Debye temperature curves for the two models show the same characteristic as those of copper, namely, Model II gives better result in low temperatures while Model I gives better result (which approaches to a constant value), at higher temperatures (Fig. 6-10). Except for the 0°K point the experimental ω's are from the work of Giauque and Meads [49] corrected for the electronic contribution [50]. The 0°K value is due to Phillips [50].

**Nickel**

Model II gives reasonably good result of dispersion curves of nickel (Fig. 6-12) except the longitudinal dispersion curves in the [$\zeta \zeta$] direction. This result is better than that provided by Model I. (Fig. 6-11).

The frequency spectrum of nickel in Model II has a broad peak in the range of frequency between $4.5 \times 10^{12}$ cps and $6 \times 10^{12}$ cps, and a sharper and higher peak at about 8.3 cps (Fig. 6-14). This is in good agreement with that calculated by Birgeneau et al. [37] using a fourth-neighbour tensor-force model, and the experimental results obtained by Tchernoplekov et al. [51], Brugger [52], and Mozer et al. [53]. The spectrum provided by Model I is not so encouraging. (Fig. 6-13).
Fig. 6-11 Nickel (AFM - 1, 296°K)

REDUCED WAVE VECTOR PARAMETER, $\xi = a k_i$
Reduced wave vector parameter, $\xi = a k_1$

Fig. 6-12. Dispersion curves of Nickel by AFM-II at 296°K.
Fig. 6.15. Debye temperature of Nickel.
The "experimental" curve for Debye temperatures shown in Fig. 6-15 represents the experimental heat capacity data of Busey and Giauque [54] and of Rayne and Kemp [55] as interpreted by the latter authors. The analysis of heat capacity ($C_V$) data for nickel is complicated by the existence of a magnetic contribution $C^m$, in addition to the usual conduction electron ($C^e$) and lattice ($C^l$) terms. Thus an analysis of $C_V(T)$ for $T < 10^0 K$ by means of the formula,

$$C_V = C^e + C^l = \sqrt{T} + gT^3$$

is quite inadequate in the case of nickel. In the absence of a magnetic field, the dominant term [56] in $C^m$ is of the form $AT^{3/2}$ for low $T$. The existing $C_V$ data for nickel are not sufficiently precise to determine the value of $A$. This can be found, however, from saturation magnetization measurements, and the appropriate allowance for $C^m$ made in the analysis of $C_V$. In this way, Rayne and Kemp [55] have deduced the "experimental" curve shown in Fig. 6-15. Model II provides reasonable result in comparison with the experimental curve. This theoretical curve tends to a constant at higher temperature. On the other hand at temperatures higher than $260^0 K$, it seems that the results by Model I are in better agreement.

As a conclusion, we find that the angular force Model II provides reasonably good results for dispersion curves, frequency spectra, and Debye temperatures. Though only four force parameters are used, the results
are comparable to those obtained from models with more parameters.

The histograms and Debye temperatures for copper and aluminum
were calculated from the force constants at 0°K. It is possible that
the disagreement with Debye temperatures at high temperatures could be
lessened if force constants appropriate to those temperatures are used.

(2) **Body-centered cubic lattice** -

Upon equating the secular equation (3.20) and the secular
equation of a second neighbour tensor-force model for the b.c.c. lattice
(see footnote in p. 74), we find that, as far as the frequency is concerned,
the angular force Model I for b.c.c. lattice is equivalent to the second-
neighbour tensor-force model with the following identities,

\[
\frac{4}{3} (a_1 + 2n_1) = a_1^{111} \tag{6.26}
\]

\[
a_2 = a_1^{200} \tag{6.27}
\]

\[
n_2 = a_2^{200} \tag{6.28}
\]

and

\[
\frac{1}{3} (a_1 - n_1) = b_1^{lll} \tag{6.29}
\]

which

The angular force Model II for b.c.c. lattice also involves 4
constants is equivalent to the second neighbour tensor-force model with
the following identities,

$$\frac{\alpha_1}{3} + \frac{16\nu_1}{9a^2} + \frac{8\nu_2}{3a^2} = \alpha_1$$  \hspace{1cm} (6.30)

$$\alpha_2 + \frac{32\nu_1}{9a^2} = \alpha_1$$  \hspace{1cm} (6.31)

$$-\frac{8\nu_1}{9a^2} + \frac{4\nu_2}{3a^2} = \alpha_2$$  \hspace{1cm} (6.32)

$$\frac{\alpha_1}{3} - \frac{8\nu_1}{9a^2} + \frac{4\nu_2}{3a^2} = \beta_1$$  \hspace{1cm} (6.33)

If in equation (3.20), we use \(\alpha_1\), \(\alpha_1\), \(\alpha_2\) and \(\beta_1\) as the parameter instead of \(\alpha_1\), \(\alpha_2\), \(\eta_1\), \(\eta_2\), that is, by substituting (6.26), (6.27), (6.28) and (6.24) into (3.20), we get a secular equation which would be identical to that obtained by substituting \(\alpha_1\), \(\alpha_1\), \(\alpha_2\) and \(\beta_1\) into equation (4.50). From this, it is obvious that the two angular force models are equivalent as far as the frequency spectrum is concerned.

An examination of Tables 6 and 7 in Chapter V, shows that in both models, in general, the first neighbour force parameter \(\alpha_1\), is of magnitudes two or three times those of the second neighbour force parameter
\( \alpha_2 \). In the case of molybdenum in Model II the values of \( \alpha_2 \) are larger than those of \( \alpha_1 \). The signs of the values of \( \alpha_1 \) and \( \alpha_2 \) in both models are positive.

In general, the values of the angular force parameters, \( \eta_1 \) or \( \mu_1/a^2 \) are smaller than \( \alpha_1 \) by a factor of thirty or forty. \( \eta_1 \) values are greater than \( \eta_2 \) values and \( \mu_1/(a^2) \) values are greater than \( \mu_2/(a^2) \) values with the exception for Ta. In general, the values of \( \eta_1 \) are greater than those of \( \mu_1/(a^2) \) and the values of \( \eta_2 \) are greater than those of \( \mu_2/(a^2) \).

In the cases of molybdenum, tungsten and iron, the values of \( \mu_2/(a^2) \) are around one-tenth of those of \( \mu_1/(a^2) \) and are negligible in comparison with those of \( \alpha_1 \). This is why Clark et al. [23] have obtained reasonable result for dispersion curves of iron, by means of a three constant angular force model.

The signs of \( \eta_1 \) are all negative. The signs of \( \eta_2 \) and \( \mu_2/(a^2) \) are all positive except those for tantalum. The signs of \( \mu_1/(a^2) \) are all negative except those for tantalum.

The magnitude and signs of the angular force parameters of tantalum show that its behaviour is different from the other metals considered here.

**Sodium**

The dispersion curves of sodium in Fig. 6-16 are in good accord with the experimental results of Woods et al [42].
Fig. 6-16. Dispersion curves of sodium at 90°K.
Fig. 6-17. Frequency Spectra of sodium.
The frequency spectrum of sodium in Fig. 6-17 has a peak at about $1.7 \times 10^{12}$ cps, a higher one at $2.6 \times 10^{12}$ cps and a highest one at $3.6 \times 10^{12}$ cps. This is in good agreement with that obtained by Dixon Woods and Brockhouse [57] using a fifth-neighbour tensor-force model.

The experimental points of Debye temperatures shown in Fig. 6-18 were derived by Dixon et al. [57] from experimental heat capacity data of Martin [58]. The theoretical Debye temperature curve shows better agreement with experimental values at temperatures below $100^\circ$K. For higher temperatures, the theoretical value increases with increasing temperature while the experimental value decreases.

**Tantalum**

The dispersion curves of Tantalum have been measured by Woods [43].

The transition metals show a number of perplexing properties and it is also reflected in their measured dispersion curves, which are known to be quite complicated. It is therefore not surprising that in the case of tantalum, theoretical curves do not show a good agreement with the experimental results. In the [100] direction, for $\xi > .5$ the longitudinal branch takes a dip and goes below the transverse branch. It is not possible to reproduce such a behaviour with only four force constants.

We have mentioned earlier the discordance of the magnitude and
REDUCED WAVE VECTOR PARAMETER, $\zeta = \alpha k_i$

FIG. 6-19 Tantalum ($296^\circ$K)
Fig. 6-20.
signs of the force constants of tantalum in comparison with other metals.

The frequency spectrum of tantalum has one peak at $2.8 \times 10^{12}$ cps and a higher and sharper peak at $5.2 \times 10^{12}$ cps (Fig. 6-20). Its shape is similar to that obtained by Woods [43], calculated from the seventh-neighbour general force model.

Heat capacity measurements on tantalum have been carried out by Clusius and Losa [59]. The experimental points for $\theta_1$'s were obtained by subtracting the electronic heat capacity from their results. A number of values of $\gamma$ have been proposed. A majority of them are close to $1.4 \times 10^{-4}$ cal/°G. at. deg.$^2$ (Gschneider [60]) and this value was also adopted here.

The theoretical Debye temperature curve (Fig. 6-21) has reasonable agreement with the experimental values for temperatures below 100°K. For higher temperatures, the experimental value increases rapidly with increasing temperature, while the theoretical value remains almost constant. It appears that the value of $\gamma$ used here is not completely satisfactory.

Molybdenum

The dispersion curves of molybdenum (Fig. 6-22) in the direction [001] have better agreement with the experimental values [44] than that of the dispersion curves in the other directions.

The frequency spectrum of molybdenum has a sharp peak at
Fig. 6-22. Dispersion curves of Molybdenum (296°K)
Fig. 6-24. Debye temperature of Molybdenum.
$5.1 \times 10^{12}$ cps and a lower one at $8.5 \times 10^{12}$ cps. (Fig. 6-23).

The Debye temperature curve of molybdenum agrees with experimental values for temperatures lower than $100^\circ$K (Fig. 6-24). At higher temperatures, the theoretical value increases gradually with increasing temperature, while the experimental value fluctuates.

The experimental values were derived from the heat capacity measurements of Clusius and Franzosini [61] using $\gamma = 5.02 \times 10^{-4}$ cal/(g-at. deg.$^2$) (Gschneider [60]).

**Tungsten**

The dispersion curve of tungsten show better agreement with experimental points in the [001] direction than in the others. (Fig. 6-25). The experimental values have been obtained by Chen and Brockhouse [45].

The histograms of tungsten has a sharp peak at $4.1 \times 10^{12}$ cps and a lower one at $6.7 \times 10^{12}$ cps (Fig. 6-26).

The Debye temperature curves of tungsten shows reasonable agreement with the experimental values. For temperature higher than $200^\circ$K, the theoretical value remains constant while the experimental value decreases with increasing temperature.

The experimental values were obtained from the heat capacity measurements of Clusius and Franzosini [61] using $\gamma = 2.92 \times 10^{-4}$ cal/g-at. deg.$^2$) (Gschneider [60]).
Fig. 6-25 Tungsten (room temperature)
Fig. 6-26. Frequency spectra for Tungsten.
Iron

The dispersion curves of iron (Fig. 6-28) are in good agreement with the experimental points obtained by Low [41].

The frequency spectrum of iron has a plateau in the frequency range $4.5 \times 10^{12}$ cps to $7.5 \times 10^{12}$ cps and a sharp peak at $9 \times 10^{12}$ cps (Fig. 6-29).

As in the case for nickel, the specific heat of iron has a spin-wave contribution ($a T^{3/2}$) in addition to the usual conduction electron ($\gamma T$) and lattice terms. Different experimenters have found somewhat different values of $a$ and $\gamma$. Recent experiments of Dixon et al. [62] give $\gamma = (11.34 \pm 0.03) \times 10^{-4}$ cal/mole deg$^2$ and $a = (1.15 \pm 0.09) \times 10^{-5}$ cal/mole deg$^{5/2}$. Mahesh and Dayal [63] have used these values of $a$ and $\gamma$ to derive Debye temperatures from the experimental values of $C_v$ measured by Dmyckaerts [64] and Kelley [65]; these experimental values are reproduced in Fig. 6-30. The theoretical curve is very similar to that calculated by Mahesh and Dayal [63] by using an extended Krebs model [66]. The agreement between the experimental values and the theoretical curve is not unsatisfactory.

In conclusion we find that for those metals whose dispersion curves are not complicated (e.g. Na, Fe) the second-neighbour tensor-force model can be used with fair success. For others though it may not be very satisfactory for the dispersion curves, it still can give a reasonable description of the average frequency spectrum and specific heat.
Fig. 6-28, Iron (289°K)
Fig. 6-30. Debye temperature of Iron.
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