NEUTRON SCATTERING STUDIES
OF
LATTICE VIBRATIONS IN B.C.C. METALS

BY

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McMaster University
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Scope and contents:

The frequency - wave vector dispersion relations of the lattice vibrations in the symmetry directions of body centred cubic iron at room temperature have been measured by means of neutron inelastic scattering. An analysis in terms of Born-Von Karman general forces is reported. Forces to third neghbours are required to obtain a fit. Forces probably exist beyond fifth neghbours. The force system could be axially symmetric. The forces between first neighbours are found to be attractive if considered as arising from a potential.

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INTRODUCTION

The energy of the thermal neutrons is of the same order as that of the lattice vibrations. So when the thermal neutrons pass through a crystal, the energy gained or lost by neutrons can be measured and give valuable informations about the dispersion relations for the normal mode vibrations. This makes the thermal neutrons as a tool for studying the dispersion relations and the frequency spectrum preferable to x-rays. This can be seen directly if we know that in the case of scattering of x-rays by lattice vibrations, the energy of the x-rays is so much larger than the energy of the lattice vibrations that the relative energy exchange between radiation and lattice is negligible.

The energy of the thermal neutrons is of the order of magnitude of 0.1 eV which corresponds to a de Broglie wave length of the order of interatomic spacings in crystals. As a result of striking the scattering centres in the crystal lattice by the neutron wave, the scattered waves interfere. There is the coherent scattering and the inchoherent scattering. If the neutrons are scattered by nuclei with no spin and no isotopes, the interference is greatest and it is in this case coherent. If the neutrons are scattered by nuclei with isotopes and spin randomly dispersed through out the crystal, the interference will be incoherent because they tend to scatter independently of each other.

In studying a specimen using thermal neutrons, the atoms composing the crystal should have good nuclear properties. i.e. the incoherent scattering cross-section 6_{inc} should be small. Due to their high capture cross-sections Lithium and Silver may be among the difficult subjects to study the thermal nuetrons (Brockhouse 66). Because of the large incoherent spin scattering cross-section of Hydrogen, one should be sure that his specimen is free from it. Because of the fact that the scattering cross section is inversely proportional to the frequency, the frequencies should not be too high.

Iron which we studied is one of the elements which have good nuclear properties.

Chapter I

General Theory :-

A solid is actually a discrete lattice. Consider a crystal composed of an infinite number of unit cells. Each cell is bounded by three noncoplanar vectors a_1, a_2, a_3. Let each unit cell contains n atoms. Locate an origin at some atom so that we can denote the equilibrium position vector of the $\ell^{\underline{th}}$ unit cell relative to this origin by

$$\bar{R}_\ell = \ell_1 a_1 + \ell_2 a_2 + \ell_3 a_3 \tag{1}$$

ℓ_1, ℓ_2 and ℓ_3 are integers.

where a_1, a_2 and a_3 are the primitive translation vectors of the lattice. The locations of the n atoms within the unit cell are given by the vectors R(k), k distinguishes the different atoms in the unit cell and takes the values 0, 1, ..., n-1.

Let us choose the origin of coordinates in such a way that $R(k = 0) = 0$

$\therefore$ In general the position vector of the $k^{\underline{th}}$ atom in the $\ell^{\underline{th}}$ unit cell is given by:

$$\bar{R}\binom{\ell}{k} = \bar{R}(\ell) + \bar{R}(k) \tag{2}$$

Each atom is displaced from its equilibrium position by the amount $\bar{U}\binom{\ell}{k}$ as a result of thermal fluctuations.

$\therefore$ The total kinetic energy of the lattice becomes

$$T = \frac{1}{2}\sum_{\ell,k,\alpha} M_k \dot{U}_\alpha^2\binom{\ell}{k} \tag{3}$$

M_k is the mass of the k<u>th</u> atom.

$U_\alpha\binom{\ell}{k}$ is the α-cartesian component of $\bar{U}\binom{\ell}{k}$

$\alpha = x, y, z.$

The total potential energy Φ of the crystal is a function of the instantaneous positions of all atoms.

Expanding Φ in powers of $\bar{U}\binom{\ell}{k}$, we have

$$\Phi = \Phi_0 + \sum_{\ell,k,\alpha} \Phi_\alpha\binom{\ell}{k} U_\alpha\binom{\ell}{k} + \frac{1}{2}\sum_{\substack{\ell,k,\alpha \\ \ell',k',\beta}} \Phi_{\alpha\beta}\binom{\ell\ell'}{kk'} U_\alpha\binom{\ell}{k} U_\beta\binom{\ell'}{k'} + \ldots \tag{4}$$

In the harmonic approximatioh, we neglect higher order terms.

Φ_0 = the static potential energy of the crystal

$$\Phi_\alpha\binom{\ell}{k} = \left.\frac{\partial\Phi}{\partial U_\alpha\binom{\ell}{k}}\right]_0 \tag{5}$$

$$\Phi_{\alpha\beta}\binom{\ell\ell'}{kk'} = \left.\frac{\partial^2\Phi}{\partial U_\alpha\binom{\ell}{k}\partial U_\beta\binom{\ell'}{k'}}\right] \tag{6}$$

The derivatives are evaluated in the equilibrium configuration.

The physical interpretation of $\Phi_{\alpha}\binom{\ell}{k}$ is that it is the negative of the force acting in the α direction on the atom at $\underline{R}\binom{\ell}{k}$ in the equilibrium configuration. So

$$\Phi_{\alpha}\binom{\ell}{k} = 0 \qquad (7)$$

because the force on any particle at the equilibrium configuration must vanish.

From equation (3), (4) and (7) and within the harmonic approximation we can write a Hamiltonian for the crystal in the form:

$$H = \Phi_0 + \frac{1}{2} \sum_{\ell k \alpha} M_k \dot{U}^2 \binom{\ell}{k} + \frac{1}{2} \sum_{\substack{\ell k \alpha \\ \ell' k' \beta}} \Phi_{\alpha\beta}\binom{\ell \ell'}{k k'} U_{\alpha}\binom{\ell}{k} U_{\beta}\binom{\ell'}{k'} \qquad (8)$$

We can define $\Phi_{\alpha\beta}\binom{\ell \ell'}{k k'}$ as the force exerted in the α-direction on the atom at $\bar{R}\binom{\ell}{k}$ when the atom at $\bar{R}\binom{\ell'}{k'}$ is displaced a unit distance in the β direction. This can be seen from the equation of motion of the lattice which takes the form

$$M_k \ddot{U}\binom{\ell}{k} = - \frac{\partial \Phi}{\partial U_{\alpha}\binom{\ell}{k}} = - \sum_{\ell' k' \beta} \Phi_{\alpha\beta}\binom{\ell \ell'}{k k'} U_{\beta}\binom{\ell'}{k'} \qquad (9)$$

if we look to equation (6), we notice that:

$$\Phi_{\alpha\beta}\binom{\ell\ell'}{kk'} = \Phi_{\beta\alpha}\binom{\ell'\ell}{k'k} \qquad (10)$$

The way the lattice is defined shows that if the lattice as a whole is translated relative to itself by a lattice vector $R(\ell)$ it coincides with itself. i.e. the lattice is periodic i.e. the periodicity of the lattice requires that $\Phi_{\alpha}\binom{\ell}{k}$ to be independent of ℓ. while $\Phi_{\alpha\beta}\binom{\ell\ell'}{kk'}$ depends on the relative cell index $\ell-\ell'$ and not on ℓ & ℓ' separately. This means that:-

$$\left.\begin{aligned} &\Phi_{\alpha}\binom{\ell}{k} = \Phi_{\alpha}\binom{0}{k}, \\ &\Phi_{\alpha\beta}\binom{\ell\ell'}{kk'} = \Phi_{\alpha\beta}\binom{\ell-\ell'}{kk'} \end{aligned}\right\} \qquad (11)$$

Equations (9), the equations of motion, form an infinite set of simultaneous linear differential equations. Suppose a solution of the form:

$$U_{\alpha}\binom{\ell}{k} = \frac{1}{\sqrt{M_k}} U_{\alpha}(k)\, e^{-[i\omega t - iq.R(\ell)]} \qquad (12)$$

Substituting this soln. in equation (9) making use of the periodicity of the lattice and equation (11):

$$\therefore \quad \omega^2 U_\alpha(k) = \sum_{k'\beta} D_{\alpha\beta}\binom{q}{kk'} U_\beta(k') \tag{13}$$

where $D_{\alpha\beta}$ is usually called the dynamical matrix and defined as :

$$D_{\alpha\beta}\binom{q}{kk'} = \frac{1}{\sqrt{M_k M_{k'}}} \sum_{\bar{\ell}} \Phi_{\alpha\beta}\binom{\bar{\ell}}{kk'} e^{-iq.\underline{R}(\bar{\ell})} \tag{14}$$

where $\underline{q}$ is the wave vector whose magnitude is $\left|\frac{2\pi}{\lambda}\right|$, where λ is the wave length, and $R(\bar{\ell}) = R_{\ell} - R_{\ell'}$.

Equations (13) have soln if and only if the determinant of the coefficients vanish:

i.e.

$$\left| D_{\alpha\beta}\binom{\vec{q}}{kk'} - \omega^2 \delta_{\alpha\beta} \delta_{kk'} \right| = 0 \tag{15}$$

Equation (15) is an equation of $3n^{\underline{th}}$ degree in ω^2. The 3n solns for each value of $\bar{q}$ will be denoted by $\omega_j^2(q)$, where $j = 1, 2, \ldots, 3n$.

From equation (14)

$$D^*_{\alpha\beta}\binom{q}{kk'} = D_{\beta\alpha}\binom{q}{kk'} \tag{16}$$

The 3n x 3n matrix obtained from the coefficients $D_{\alpha\beta}\binom{q}{kk'}$
Pairing
by paining the indices (α, k) and (β, k') is Hermitian.

i.e. $\omega_j^2(q)$'s are real which means $_j(q)$ is either real or purely imaginary.

The microscopic conditions for the stability of the lattice is that each $\omega_j(q)$ be positive because a purely imaginary value of $\omega_j(q)$ would imply a vibrational motion of the lattice which erupts exponentially either into the part or intothe future.

In view of equation (14) this condition imposes additional restrictions on the force constants $\Phi_{\alpha\beta}\left({\ell\ell' \atop kk'}\right)$ whichare supposed to be satisfied.

The 3n functions $\omega_j^2(q)$ for each value of $\bar{q}$ can be regarded as branches of a multivaluedfunction $\omega(q)$.

$$\omega = \omega_j(q) \qquad j = 1, 2, \ldots, 3n \tag{17}$$

is called the dispersion relation.

$\omega_j(q)$ does nothave a closed expression in general. But such experessions can exist for special simple models. There exists a vector $\underline{e}\,(k \mid {q \atop j})$ for each of the 3n values of $\omega_j^2(q)$. The components of this vector are the solns to theset of equations (13) . Equations (13) can now be written in the form

$$\omega_j^2(\bar{q})\; e_\alpha\left(k \middle| {q \atop j}\right) = \sum_{k',\beta} D_{\alpha\beta}\left({q \atop kk'}\right)\; e_\beta\left(k' \middle| {q \atop j}\right) \tag{17}$$

$\bar{e}(k, {q \atop j})$ is defined through equation (17) within a constant factor. This constant factor can be chosen in such a way so that $\bar{e}\,(k|{q \atop j})$ satisfies theorthonormality conditions i.e.

$$\sum_{k,\alpha} e^{*}_{\alpha}\left(k\Big|{q \atop j}\right) e\left(k\Big|{q \atop j'}\right) = \delta_{jj'} \qquad (18)$$

$$\sum_{j} e^{*}_{\beta}\left(k'\Big|{q \atop j}\right) e_{\alpha}\left(k\Big|{q \atop j}\right) = \delta_{\alpha\beta}\,\delta_{kk'} \qquad (19)$$

Also from equation (14) which defines the dynamical matrix that :

$$D_{\alpha\beta}\left({-q \atop kk'}\right) = D^{*}\left({q \atop kk'}\right) \qquad (20)$$

If we take the complex conjugate of equation (17) and from the fact that $\omega_j^2(q)$ is always real, then from equation (20), we find that

$$e_{\alpha}\left(k\Big|{q \atop j}\right) = e^{*}\left(k\Big|{-q \atop j}\right) \qquad (21)$$

i.e. we can write : $\omega_j^2(q) = \omega_j^2(-q)$ (22)

The eigenvectors $\bar{e}\left(k\big|{q \atop j}\right)$ are real for Bravais lattices. They can be complex only for lattices made up of unit cells which contain more than one atom.

We have now an eigenvalue problem. The eigenvalues of the dynamical matrix $D_{\alpha\beta}\left({q \atop kk'}\right)$ are $\omega_j^2(q)$ which will be identified as the squares of the normal mode frequencies of the crystal.

It can be shown that three of the 3n solns for each q go to zero as q goes to zero. Such modes are called acoustic modes, since the n particles in each unit cell move in parallel and with equal amplitudes which is the characteristic of the displacement in an elastic continuum upon which a sound wave is impressed.

The 3n-3 modes whose frequencies do not vanish at q=0, are called optical modes. The reason it is called optical modes may have been arised from the circumstances that for ionic crystals of NaCl type, the two ions in each unit cell vibrate 180° out of phase, while the centre of mass of the cell remains fixed. A net fluctuating dipole moment for the crystal is induced by these modes of vibration. This is true since the two ions have charges of opposite sign. This dipole moment can interact with an external electromagnetic field.

In the case of the acoustic modes, in the limit of infinitely long waves, the atoms in a unit cell move in parallel with zero frequency.

For every small but finite values of the wave vector $\bar{q}$ this is still approximately true, i.e. the displacements of the atoms in a unit cell are nearly equal and the corresponding three frequencies for a given q are small. The low frequency vibrations correspond to sound waves in the crystal.

We have now two approaches:

(1) The frequencies of sound waves in a solid are determined by the macroscopic elastic constants of the solid.

(2) The frequencies of all the modes in a crystal are determined by the atomic force constants $\Phi_{\alpha\beta}\binom{\ell\ell'}{kk'}$.

From these two approaches, there must exist relations between the $\left\{\Phi_{\alpha\beta}\binom{\ell\ell'}{kk'}\right\}$ and the elastic constants $\left\{c_{ijk\ell}\right\}$.

If we examine the equations of motion in the limit as $q \rightarrow 0$ and Compare them with the corresponding equation from the theory of elasticity we can obtain~~d~~ these relations.

This was treated by Born and Huang (1954).

The explicit relations between the atomic force constants and the elastic constants for simple models of the primitive cubic lattices has been worked out by De Launay.

From the theory of elasticity the secular equation by which the possible frequencies are related to the elastic constants is (De Launay, 1956)

$$\begin{vmatrix} (c_{11}-c_{44})q_1^2+c_{44}q^2+4\pi^2\rho\nu^2 & (c_{12}+c_{44})q_1q_2 & (c_{12}+c_{44})q^2 \\ (c_{12}+c_{44})q_1q_2 & (c_{11}-c_{44})q_2^2+c_{44}q^2-4\pi^2\rho\nu^2 & (c_{12}+c_{44})q_2q_3 \\ (c_{12}+c_{44})q_1q_3 & (c_{12}+c_{44})q_2q_3 & (c_{11}-c_{44})q_3^2+c_{44}q^2-4\pi^2\rho\nu^2 \end{vmatrix} = 0 \tag{23}$$

Since dispersion is absent for sufficiently long waves.

The velocity of sound is given by $U = \frac{2\pi\nu}{q}$. If the wave is parallel to the [100] direction

$$\therefore \quad q_1 = q, \quad q_2 = q_3 = 0$$

substituting in the equations of motion taking the components of the wave vector along the symmetry directions [100] , [110] , [111] , we find that the longitudinal velocity U_ℓ is given by

$$\rho U_\ell^2 = c_{11} \qquad (24)$$

The velocity of plane transverse waves is given by

$$\rho U_t^2 = c_{44} \qquad (25)$$

in case of a wave parallel to the [110] direction

$$q_1 = q_2 = q/\sqrt{2} \, , \; q_3 = 0 \qquad ($$

This gives

$$\rho U_\ell^2 = (c_{11}+c_{12} +2c_{44})/2 \qquad (26)$$

$$\rho U_t^2 = c_{44} \qquad (27)$$

where here U_t is the velocity of a transverse wave polarized parallel to the z-axis

and

$$\rho U_t'^2 = (c_{11}-c_{12})/2 \qquad (28)$$

where $U_t'^2$ is the velocity of a transverse wave polarized perpendicular to the z-axis.

in the case of a wave parallel to the [111] direction

$$q_1 = q_2 = q_3 = q / \sqrt{3} \qquad (29)$$

$$\rho U_\ell^2 =(c_{11} + 2c_{12} + 4c_{44})/3 \qquad (30)$$

and

$$\rho U_t^2 = (c_{11}-c_{12}+c_{44})/3 \tag{31}$$

It can be shown also that, the quantity

$$S = \frac{c_{11} - c_{12}}{2\,c_{44}} \tag{32}$$

is unity if the material is elastically isotropic. This is true only for tungston among elements which has cubic structure. It can be also shown (Stokgold) that if the interactions between the atoms of a monatomic crystal are described by central forces, certain relations exist between the elastic constants

e.g. in the cubic crystals

$$c_{12} = c_{44} \tag{33}$$

which is known as the Cauchy relation.

The values which the wave vector $\bar{q}$ can assume have to be determined by the boundry conditions imposed on the components of the displacement vectors $\bar{\bar{U}}\,(\begin{smallmatrix}\ell\\k\end{smallmatrix})$. Born and Von-Karman introduced the cyclic boundry conditions; It can be formulated as follows. Consider an infinitely extended crystal subdevided into "macrocrystals" each of which contains LxLxL=N unit cells. These macrocrystals fill all space, and are parallelpipeds whose edges are defined by the vectors La_1, La_2, La_3.

Regard any one of the macrocrystals as the physical crystal whose vibrational properties we are studying. According to the cyclic Boundary condition, the atomic displacements are considered to be periodic with the periodicity of the macrocrystals

i.e. $$\bar{U}\binom{\ell+L}{k} = \bar{U}\binom{\ell}{k} \tag{33}$$

The cyclic boundary condition simplifies the derivation of every result in the theory of lattice dynamics which does not depend explicitly on the crystal's surface. It also provides a convenient way of normalizing the potential and kinetic energies of a crystal to a finite volume. Now, we apply the cyclic boundary condition to the components of the displacement vector.

$$U_\alpha\binom{\ell}{k} = \frac{1}{\sqrt{M_k}} U_\alpha(k)\, e^{-[i\omega t+q.R(\ell)]} \tag{12}$$

from which, we find that

$$e^{iq.La_1} = e^{iq.La_2} = e^{iq.La_3} = 1 \tag{34}$$

Define a reciprocal lattice vector by

$$\bar{a}_i \,.\, \bar{b}_j = \delta_{ij} \tag{35}$$

where $\bar{b}_1$, $\bar{b}_2$ and $\bar{b}_3$ are the primitive translation vectors of the reciprocal lattice.

$$\bar{b}_1 = \frac{\bar{a}_2 \times \bar{a}_3}{a_1.(a_2 x a_3)}$$

$$\bar{b}_2 = \frac{\bar{a}_3 \times \bar{a}_1}{\bar{a}_1.(\bar{a}_2 x \bar{a}_3)}$$

$$\bar{b}_3 = \frac{\bar{a}_1 \times \bar{a}_2}{\bar{a}_1.(a_2 x \bar{a}_3)} \qquad (36)$$

where $v_a = \bar{a}_1.(\bar{a}_2 x \bar{a}_3)$ = the volume of a primitive unit cell of the direct lattice. In the reciprocal lattice, a lattice vector is given by

$$\tau(h) = h_1 b_1 + h_2 b_2 + h_3 b_3 \qquad (37)$$

where h_1, h_2 and h_3 are integers.

The scaler product between a direct lattice vector and a reciprocal lattice vector is an integer.

i.e. $\bar{R}(\ell).\tau(h) = \ell_1 h_1 + \ell_2 h_2 + \ell_3 h_3$ = integer (38)

$\therefore$ The wave vector $\bar{q}$ can be given by $\bar{q} = \frac{1}{L}\tau(h) =$

$$\frac{h_1}{L}\bar{b}_1 + \frac{h_2}{L}\bar{b}_2 + \frac{h_3}{L}b_3 \qquad (39)$$

which satisfies equation (34). If we $\overset{\text{add}}{\underline{\text{aid}}}$ to $\bar{q}$ any reciprocal lattice vector $\vec{\tau}(h)$, the value of $U_\alpha\binom{\ell}{k}$ is unaffected (from equations(12) & (38)). i.e. All distinct solns are obtained if the allowed values of $\bar{q}$ lie in one unit cell of the reciprocal lattice.

i.e. $\overset{\vec{q}}{\bar{q}} = \frac{h_1}{L}\bar{b}_1 + \frac{h_2}{L}\bar{b}_2 + \frac{h_3}{L}\bar{b}_3$

$$\text{where } h_1, h_2, h_3 = 1, 2, \ldots, L \;.. \qquad (40)$$

i.e. we have $N = L^3$ allowed values of $\overset{\vec{q}}{\cancel{k}}$. where N is the number of unit cells in the crystal. $\overset{h_i}{h_1}$ can be conveniently restricted to within ranges $-\frac{L}{2} \leqslant h_i \leqslant \frac{L}{2}$.

Now, the cyclic boundary condition leads to N independent $\bar{q}$ vectors which define the interior and surfaces of the first Brillouin zone.

$\therefore$ In the harmonic approximation we have 3nN independent normal vibrations

$$\bar{e}(k\,|\,{}^{q}_{j})\, e^{iq\cdot\bar{R}} \qquad \begin{array}{l} k = 1, 2, \ldots n \\ j = 1, 2, \ldots n \\ q = q_1, q_2, \ldots q_n \end{array} \qquad (41)$$

with corresponding 3 nN normal frequencies $\omega_j^2(q)$.

The harmonic approximation we discussed above leads to simple results and a sharply defined phonon state and dispersion relations exist only in the harmonic approximation.

The one phonon peak in the inelastic neutron scattering is sufficiently narrow for temperatures well below the melting point of metals. The existence of well defined phonons is a physical reality which justifies the use of the harmonic approximation as a starting point of an analysis of lattice vibrations in metals. Since phonons are the quantized thermal vibration of ions in a crystal lattice, we have to quantize the lattice vibrations to have a description in terms of phonons.

Let us start by expanding $U_\alpha \binom{\ell}{k}$ in terms of plane waves

$$U_\alpha \binom{\ell}{k} = \frac{1}{\sqrt{NM_k}} \sum_{\bar{q},j} e_\alpha \left(k \,|\, {q \atop j}\right) Q \binom{q}{j} e^{i\bar{q}.\bar{R}(\ell)} \tag{42}$$

$Q\binom{q}{j}$ must satisfy the reailty condition

$$Q \binom{-\bar{q}}{j} = Q^{*} \binom{\bar{q}}{j} \tag{43}$$

that is because $U_\alpha \binom{\ell}{k}$ is real. The K.E. becomes :

$$T = \frac{1}{2N} \sum_{\ell k \alpha} \sum_{qq'} e_\alpha \left(k \,|\, {q \atop j}\right) e_\alpha \left(k \,|\, {q' \atop j'}\right) \overset{\dot{Q}}{Q'} \binom{q}{j} \dot{Q} \binom{\overset{q'}{k'}}{j'} e^{i(q+q').\bar{R}(\ell)} \tag{44}$$

But $$\sum e^{i\bar{q}.\bar{R}(\ell)} = N\Delta(\bar{q}) \tag{45}$$

where $\Delta(\bar{q})$ vanishes unless $\bar{q}$ is zero or a reciprocal lattice vector in which case it equals unity.

Since q & q' are restricted to lie in the 1st Brillouin zone their sum can only be zero in order that $\Delta(q+q')$ should not vanish

$$\therefore \quad T = \frac{1}{2} \sum_{q \atop j} \dot{Q}^{*} \binom{q}{j} \dot{Q} \binom{q}{j} \tag{46}$$

The potential energy can be shown to take the form

$$\Phi = \frac{1}{2}\sum_{\substack{q\\j}} \omega_j^2(q)\, Q^{*}\binom{q}{j}\, Q\binom{q}{j} \tag{47}$$

$\therefore$ In terms of the new coordinates the Hamiltonian of the lattice will be

$$H = \frac{1}{2}\sum_{\substack{q\\j}} \Big\{ \dot{Q}^{*}\binom{q}{j}\, \dot{Q}\binom{q}{j} + \underline{\omega^2\binom{q}{j}\, Q^{*}\binom{q}{j}}\, \varphi(q_j\cdot) \tag{48}$$

The Lagrangian L is given by

$$L = T - \Phi$$

The momentum conjugate to $Q^{*}\binom{q}{j}$ is

$$P\binom{q}{j} = \frac{\partial L}{\partial \dot{Q}^{*}\binom{q}{j}} = \dot{Q}\binom{q}{j} \tag{49}$$

$$\therefore \quad H = \frac{1}{2}\sum_{\substack{q\\j}} \Big\{ P^{*}\binom{q}{j}\, P\binom{q}{j} + \omega_j^2(q) Q^{*}\binom{q}{j} Q\binom{q}{j} \Big\} \tag{50}$$

From Hamilton's equations of motion,

$$\left.\begin{aligned} \dot{Q}\binom{q}{j} &= \frac{\partial H}{\partial P^{*}\binom{q}{j}} \\ -\dot{P}\binom{q}{j} &= \frac{\partial H}{\partial Q^{*}\binom{q}{j}} \end{aligned}\right\} \tag{51}$$

$\therefore$ The equation of motion of the coordinate $Q\binom{q}{j}$ is

$$\ddot{Q}\binom{q}{j} + \omega_j^2(q)\, Q\binom{q}{j} = 0 \qquad (52)$$

Each of the new coordinates is a periodic function which involves only one of the frequencies $\omega_j(q)$.

Equation (50) is a sum of 3nN independent harmonic oscillator hamiltonian. After treating this collection of oscillators quantum mechanically, the total vibrational state of the crystal is given by

$$\Phi_q\left(\{n_j(q)\}\right) = \prod_{q,j} | n_j(q) \rangle \qquad (53)$$

with the total energy

$$\begin{aligned}\mathcal{E}_q\left(\{n_j(q)\}\right) &= \sum_{q,j} \epsilon_{n_j}(q) \\ &= \sum_{q,j} \left\{n_j(q) + \tfrac{1}{2}\right\} \hbar\, \omega_j(q) \qquad (54)\end{aligned}$$

$n_j(q)$ is the occupation number of the oscillator state (j,q). The vibrating lattice is transformed into an assembly of 3nN independent harmonic oscillators.

The independent oscillator state (j,q) is called a phonon state. The energy of a single phonon in this state is $\hbar\omega_j(q)$.

$\omega_j(q)$ can be identified as that obtained by the dynamical matrix mentioned above.

The creation and annihilation operators of a phonon state are defined by the following relations (Maradudin et al.):

$$a^{*}_{q,j} = \frac{P^{*}\binom{q}{j}}{\sqrt{2\hbar\,\omega_j\,(q)}} + \sqrt{\frac{\omega_j(q)}{2\hbar}}\,Q^{*}\binom{q}{j}$$

$$a_{q,j} = \frac{iP\,\binom{q}{j}}{\sqrt{2\hbar\,\omega_j\,(q)}} + \sqrt{\frac{\omega_j(q)}{2\hbar}}\,Q^{*}\binom{q}{j}$$

So that

$$Q\binom{q}{j} = \sqrt{\frac{\hbar}{2\,\omega_j(q)}}\left[a^{*}_{-q,j} + a_{q,j}\right]$$

$$P\binom{q}{j} = i\sqrt{\frac{\hbar\quad{}_j(q)}{2}}\left[a^{*}_{-q,j} - a_{q,j}\right]$$

$Q\binom{q}{j}$ and $P\binom{q}{j}$ are conjugate canonical coordinate and Momentum. They satisfy the following commutation relations:-

$$\begin{aligned}
\left[Q^{*}\binom{q}{j},\ P\binom{q'}{j'}\right] &= i\hbar\,\Delta\,(q-q')\,\delta_{jj'} \\
\left[Q\binom{q}{j},\ P^{*}\binom{q'}{j'}\right] &= i\hbar\,\Delta\,(q-q')\,\delta_{jj'} \qquad (57) \\
\left[Q^{*}\binom{q}{j},\ Q\binom{q'}{j'}\right] &= \left[P^{*}\binom{q}{j},\ P\binom{q'}{j'}\right] = 0
\end{aligned}$$

Also $a_{q,j}$ & $a^{*}_{q,j}$ satisfy the following commutation relations :

$$\left[a_{q,j} \, , \, a^{*}_{q',j'} \right] = \Delta(q-q') \, \delta_{jj'}$$

$$\left[a_{q,j} \, , \, a_{q',j'} \right] = \left[a^{*}_{q,j'} \, , \, a^{*}_{q',j'} \right] = 0 \tag{58}$$

The phonon Hamiltonian can be written in terms of $a_{q,j}$ & $a^{*}_{q,j}$ in the following expression

$$H = \sum_{q,j} \hbar \, \omega_j(q) \left[a^{*}_{q,j} \; a_{q,j} + \frac{1}{2} \right]$$

$$= \sum_{q,j} \hbar \, \omega_j(q) \left[n_j(q) + \frac{1}{2} \right] \tag{59}$$

This follows from the matrix elements

$$\begin{aligned} \langle n_j(q) \,|\, a_{q,j} \,|\, n_j(q) + 1 \rangle &= \sqrt{n_j(q) + 1} \\ \langle n_j(q) + 1 \,|\, a^{*}_{q,j} \,|\, n_j(q) \rangle &= \sqrt{n_j(q) + 1} \\ \langle n_j(q) \,|\, n_{j'}(q') \rangle &= \Delta(\underline{q} - \underline{q}') \, \delta_{jj'} \end{aligned} \tag{60}$$

It can be shown that at last we end with

$$\underline{U}\binom{\ell}{k} = \sum_{q,j} \sqrt{\frac{\hbar^2}{2NM_k \hbar \, \omega_j(q)}} \left\{ a_{q,j} \, \underline{e}\left(k \middle| \begin{smallmatrix} q \\ j \end{smallmatrix}\right) e^{iq.\bar{R}_\ell} + a^{*}_{q,j} \, \overset{*}{e}_{q,j} \, e^{-iq.\bar{R}_\ell} \right\} \tag{61}$$

The total energy of the system is given by

$$E = \Phi_0 + E_0 + \mathcal{E} \tag{62}$$

where

$(\Phi_0 + E_0)$ is a constant term and

Φ_0 = the energy of the static lattice

E_0 = the zero point energy $= \frac{1}{2}\sum_{q,j} \hbar\,\omega_j(q)$

$$\mathcal{E} = \sum_{q,j} \frac{\hbar\,\omega_j(q)}{e^{\frac{\hbar\,\omega_j(q)}{k_B T}} - 1} = \sum_{q,j} \frac{\hbar\,\omega_j(q)}{e^{\beta\hbar\,\omega_j(q)} - 1}$$

$$= \sum_{q,j} \bar{n}_j(q)\,\hbar\,\omega_j(q) \tag{63}$$

where the Bose - Einstein distribution function $\bar{n}_j(q)$ is defined as :

$$\bar{n}_j(q) = \frac{1}{e^{\beta\hbar\,\omega_j(q)} - 1} \tag{64}$$

and the constant volume specific heat is derived from the energy by :

$$C_V = \left(\frac{\partial\mathcal{E}}{\partial T}\right)_V = k_B \sum_{q,j} \frac{\left\{\beta\hbar\,\omega_j(q)\right\}^2 e^{\beta\hbar\omega_j(q)}}{\left\{e^{\beta\hbar\,\omega_j(q)} - 1\right\}^2} \tag{65}$$

The above summation is replaced by an integration by introducing the frequency distribution function $g(\omega)d\omega$ which is the number of normal modes having frequency in the interval $(\omega, \omega + d\omega)$ so that :

$$\int_0^{\omega_m} g(\omega)\, d\omega = 3\, n\, N \qquad (66)$$

where ω_m is the maximum vibrational frequency of the lattice. It can be shown that in terms of $g(\omega)$ equation (65) can be replaced by :

$$C_V = k_B \int_0^{\omega_m} g(\omega) \frac{(\beta\hbar\omega)^2\, e^{\beta\hbar\omega}}{\left\{e^{\beta\hbar\omega} - 1\right\}^2}\, d\omega \qquad (67)$$

in the debye approximation (De Launay), $g(\omega)$ takes the value

$$g(\omega) = \frac{9\, n\, N}{\omega_m^3}\, \omega^2 \qquad (68)$$

where a Debye temperature θ_D is defined so that :

$$\hbar\, \omega_m = k_B\, \theta_D \qquad (69)$$

of course k_B is the Boltzman constant so that :

$$C_V = \frac{9\, n\, N\, k_B}{x^3} \int_0^{x} \frac{\xi^4\, e^{\xi}}{(e^{\xi} - 1)^2}\, d\xi \qquad (70$$

$$x = \frac{\hbar\omega_m}{k_B T} = \frac{\theta_D}{T}$$

Equation (70) gives C_V = constant at sufficiently high temperature which is the Duling - petit value while at low temp. equation (70) will give C_V as :

$$C_V = \frac{12 \pi^4 R}{5} \left(\frac{T}{\theta}\right)^3 = 464.3 \left(\frac{T}{\theta}\right)^3 \frac{\text{cal.}}{\text{deg. at. wgt.}} \qquad (71)$$

Equation (71) is the well known T^3 low (see De Launay, 1956 --- solid state physics volume 2).

Chapter II

Scattering of Thermal Neutrons :-

As we explained in the introduction, thermal neutrons can be scattered by solids either coherently or incoherently. Also neutrons do not interact strongly with the system. The neutron has a mass of the order of atomic masses, so a slow neutron has a reasonable chance, in collision with a system of atoms, of picking up or losing quanta of any of the characteristic energies of the system. We pointed out in the introduction how the changes in energy of the scattered neutrons are relatively large and easily measurable. Having a short wave length, the neutron responds to all kinds of motion in the specimen not just to those motions in which large numbers of atoms move together as in the scattering of light.

A process in which the atomic system goes from a vibrational state n to n' while the neutron is scattered from wave vector k_o to wave vector k' is governed by a differential cross-section given by: (Powell & Craseman 61):

$$\frac{d^2\delta}{d\Omega\, dE'} = \left(\frac{m_N}{2\pi\hbar^2}\right)^2 \frac{k'}{k_o} \left|F(Q)\right|^2 \sum_{n,n'} g_n \left|\sum_{\ell=1}^{N} \langle n' \left| e^{iQ.R_\ell} \right| n \rangle \right|^2 \left(\frac{\hbar^2 k^2}{2m_N} + \mathcal{E}_{n'} - \frac{\hbar^2 k_o^2}{2m_N} - \mathcal{E}_n\right) \qquad (1)$$

$$F(Q) = \int V(r)\, e^{i\underline{Q}\cdot\underline{r}}\, dr$$

= The Fourier transform of the interaction potential

g_n = the statistical wgt. of the initial vibrational

$$\text{state} = e^{-\mathcal{E}_n/k_BT} \Big/ \sum_{n'} e^{-\mathcal{E}_{n'}/k_BT} \qquad (2)$$

Fermi (1936) used a device in which he invented a δ-function potential $V(r) = \frac{2\pi\hbar^2}{m_N} b\,\delta(r)$

where $b = (\frac{A+1}{A}) b_{free}$ is the bound scattering length and A is the atomic wgt. of the scatterer so that

$$F(Q) = \frac{2\pi\hbar^2}{m_N} b$$

For elastic scattering

Letting $n' = n$, $k_o = k'$, $N = 1$ and $g_n = 1$ Substituting in equation (1)

$$\therefore \frac{d\sigma}{d\Omega} = \left(\frac{m_N}{2\pi\hbar^2}\right)^2 \left(\frac{2\pi\hbar^2}{m_N}\right)^2 b^2 = b^2$$

which is just the differential cross-section for the elastic scattering of neutrons by a single nucleus.

$\therefore$ The general expression for the differential scattering cross-section will be :

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k_o} \sum_{n,n'} g_n \left| \sum_{\ell k} \langle n' | e^{iQ.R(\overset{\ell}{k})} \, b_{\ell k} | n \rangle \right|^2 \delta(\text{Energy}) \tag{4}$$

Taking into consideration the dependence of the scattering length on the site of an atom (Isotopic or spin incoherence). Equation (4) is a general expression from which the one phonon coherent and incoherent cross-sections can be derived and will be in the form:

$$\frac{d^2\sigma_{-1}(q,j)}{d\Omega dE'} = \frac{d^2\sigma^{c}_{-1}(q,j)}{d\Omega dE'} + \frac{d^2\sigma^{inc}_{-1}(q,j)}{d\Omega dE'} \tag{5}$$

$\rightarrow d\Omega dE'$

where

$$\frac{d^2\sigma^{c}_{-1}(q,j)}{d\Omega\, dE'} = \frac{k'}{k_o} \frac{\hbar}{4\pi N} \bar{n}_j(q) \left| \sum_{\ell} e^{i(q+Q).\bar{R}_{\ell}} \right|^2$$

$$\left| \sum_{k} \bar{b}_k e^{iQ.\bar{R}_{\ell}} \frac{Q.e(k|\overset{q}{j})}{\sqrt{M_k \nu_j}} \; e^{-W(x)} \right| \delta(\text{energy}) \tag{6}$$

and

$$\frac{d^2\sigma^{inc.}_{-1}(q,j)}{d\Omega dE'} = \frac{k'}{k_o} \frac{\hbar}{4\pi} \bar{n}_j(q) \sum_{k} \frac{\sigma_{inc}}{4\pi} \frac{|Q.e(k|\overset{q}{j})|^2}{M_k \nu_j}$$

$$e^{-2W(x)} \delta(\text{energy}) \tag{7}$$

where $e^{-2W(x)}$ is called the Debye-Waller factor and

$$W(x) = \sum_{q,j} \frac{\hbar}{2NM_k \omega_j} \left| Q.e(k \tfrac{q}{j}) \right|^2 \quad (n_j(q) + \tfrac{1}{2}) \qquad (8)$$

on the thermal average $n_j(q)$ was replaced by

$$\bar{n}_j(q) = \frac{1}{e^{\beta \hbar \omega_j(q)} - 1}$$ (the Bose - Einstein distributionffunction)

Expression (7) can be simplified and the cross-sections for one - phonon creation and annihilation can be given by the expression.

$$\frac{d^2 \sigma^{c}_{\pm} (q,j)}{d\Omega \;\; dE'} = \frac{k'}{k_o} \frac{\hbar}{4\pi} \frac{(2\pi)^3}{v} \begin{Bmatrix} \bar{n}_j(q)+1 \\ \bar{n}_j(q) \end{Bmatrix}$$

$$\left| g_j(q,\tau) \right|^2 \delta(\underline{q} + \underline{Q} - \underline{G})\, \delta(E_o - E' \mp h\nu_j) \qquad (9)$$

(For N unit cells/steradian/unit Energy)

where (Brockhouse and Iyengar 58):

$$g_j(q,\tau) = \sum_k \frac{\bar{b}_k Q.\bar{e}\, (k|\tfrac{q}{j})}{\sqrt{M_k \;\; \nu_j}} \; e^{-W(x)} \;\; e^{iQ.\bar{R}_k}$$

$$E' = \frac{\hbar^2 \;\; k'^2}{2M_n} \qquad (10)$$

Integrating over E' we end with the expression (Waller & Froman 1952).

$$\frac{d\sigma^{c}_{\pm}(q,j)}{d\Omega} = \frac{k'}{k_o}\,\frac{\hbar N}{4\pi}\left\{\begin{matrix}\bar{n}_j(q)+1\\ \bar{n}_j(q)\end{matrix}\right\}\frac{g_j(q,\tau)}{|J_j|}\,\Delta(q+Q-G) \qquad (11)$$

The Jacobian J_j is given by :

$$J_j = 1 + \frac{\epsilon h}{2E'}\,(k'.\nabla_q \nu)$$

$$\epsilon = \begin{cases} 1 & \text{for phonon creation} \\ -1 & \text{for phonon annihilation} \end{cases}$$

The Jacobian depends on the slope of the dispersion curves at the point q where the phonon is being measured.

Now, the scattering of neutrons is primarily governed by the Energy transfer

$$\hbar\omega = E_o - E' \qquad (12)$$

and by the wave vector transfer

$$\bar{Q} = \bar{k}_o - \bar{k}' \qquad (13)$$

Again, there is a zero phonon process which is governed by the selection rules:

$$\left.\begin{matrix}\bar{Q} = \bar{k}_o - \bar{k}' = \bar{G} \\ \hbar\omega = E_o - E' = 0\end{matrix}\right\} \qquad (14)$$

There is also a one phonon process, in which the neutron is scattered with the creation or annihilation of one quantum. This is governed by the selection rules :

$$\bar{Q} = \bar{k}_o - \bar{k}' = \bar{G} - \bar{q} \tag{15a}$$

$$\hbar\omega = E_o - E' = \pm\hbar\omega_s \tag{15b}$$

There are also higher processes which are discussed else where (Brockhouse).

From an experimental point of view, Equations (15) together with a dispersion relation:

$\omega_s = \omega_j(q)$ constitute a system of five equations in four unknowns for which soln can be expected but rarely.

Equations (14) together with the dispersion relation, provided that $g_j(q, \ ) \neq 0$, simply says that : one would not detect any "one phonon annihilation" scattered neutrons unless there are phonons (q,j) where :

$\underline{q} = 2\pi\tau - Q$, which have exactly the energy given by

$$\Delta E = h\,\nu_j(q).$$

The dispersion relation is a property of a perticular crystal. Therefore, in general, one would not observe one phonon scattering at an arbitrary momentum and energy transfer.

Let us explain in terms of a momentum transfer given by :

$$Q^2 = k_o^2 + k'^2 - 2k_o k' \cos\varphi$$

where φ is the scattering angle.

There is another angle ψ which is the orientation angle interms of which the orientation of the crystal with respect to the incident and outgoing neutrons is characterised. k_o, k', φ and ψ are four experimentally controllable variables which are restricted by five equations in order that the scattering occurs. Usually when the chopper and time of flight method is used in an experiment, k_o, φ & ψ are fixed which means fixing the incoming neutron energy. In order to vary both the energy and momentum transfer, k' is to be changed. Varying k' over a wide range, there is no way of controlling the value of (q,j) at which the phonon is observed.
But to analyse the dispersion curves in order to obtain interatomic force constants, you would like to have dispersion relations for $\bar{q}$ in symmetry directions specially.
The so called constant Q method using the triple axis spectrometer is available (Brockhouse 61).

The Constant Q method :-

It is possible to vary the energy transfer while keeping the momentum transfer constant. In the plane of $\bar{k}_o$ and $\bar{k}_o$ which is the scattering plane the components of $\bar{Q}$ are:

$$Q_x = - k_o \sin\psi + k' \sin(\varphi + \psi)$$

$$Q_y = k_o \cos\psi - k' \cos(\varphi + \psi) \qquad (16)$$

So if one fixed k' (by fixing the analyzer angle $2\theta_A$) and for a small step incriment of k_o, φ & ψ can be varied simultaneously in small steps to keep Q_x & Q_y constant.

This is a very efficient way of measuring the dispersion curves at predetermined points in q space. The constant Q method has the following advantages (Brockhouse 61).

(1) Data are taken only in regions of reciprocal space in which they are required, thus reducing the amount of experimental work.

(2) In the conventional method, $\bar{Q}$ changes with E', and thus different neutron groups belonging to different Q's may merge. Also neutron groups are often sharper with the constant Q method than with the conventional method for the same reason.

(3) The intensities of the groups depend only on the frequency, and not (as in the conventional method) also on the gradient of the frequency, because the Jacobian $|J| = 1$ in the expression for the differential cross-section.

(4) The variation with temperature of the phonon frequency for a particular $\bar{q}$ is more easily and accurately obtainable with the constant Q method than with the conventional method. Similarly the widths of the neutron groups for different temperatures are more readily comparable.

(5) When phonons at general points in reciprocal space are to be used in the force constant analysis, it is necessary to make measurements for the 3n frequencies involved at exactly the same position in reciprocal space which is much more easily done by the constant Q than with the conventional method. With the constant Q method :

$$\left.\frac{d\sigma \pm (q,j)}{d\Omega}\right]_{Q=\text{constant}} = \frac{k' \hbar N}{k_o \, 4\pi} \begin{Bmatrix} \bar{n}_j(q)+1 \\ \bar{n}_j(q) \end{Bmatrix} \left| g_j(\tau, q) \right|^2 \Delta(q+Q-G) \tag{17}$$

and

$$\left.\frac{d\sigma \pm (q,j)}{d\Omega}\right]^{\text{Bravais lattice}}_{Q\text{-constant}} = \frac{k'}{k_o} \frac{\hbar N}{4\pi} \begin{Bmatrix} \bar{n}_j(q)+1 \\ \bar{n}_j(q) \end{Bmatrix} \frac{b^2 (Q.e(\tfrac{q}{j})^2}{M \nu_j} e^{-2W}$$

$$= \frac{\hbar}{(4\pi)^2} \frac{k'N}{k_o} \begin{Bmatrix} \bar{n}_j(q)+1 \\ \bar{n}_j(q) \end{Bmatrix} \frac{\sigma_{coh} \, (Qe(\tfrac{q}{j}))^2}{M \nu_j} e^{-2W} \tag{18}$$

which gives the differential cross-section/unit cell/steradian for the production of one phonon peak.

In equation (18), e^{-2W} is the Debye Waller factor where W was given by equation (8) and it can be simplified further for cubic crystals to give

$$W(x) = \sum_{q,j} \frac{\hbar}{2 N M k\omega_j} \left| Q.e(k|{}^{q}_{j}) \right|^2 (n_j(q) + \tfrac{1}{2}) \qquad (19)$$

which can take another form if we replace the summation by integration over the frequency distribution function to give :

$$W(k) = 3N \int_0^\infty \frac{\hbar}{2NM_k\omega_j} g(\nu) \left| Q.\bar{e}(k|{}^{q}_{j}) \right|^2 (n_j(\nu) + \tfrac{1}{2}) d\nu$$

$$= \frac{3\hbar Q^2}{4\pi M_k} \int_0^\infty d\nu \, \frac{g(\nu)}{\nu} (\bar{n}(\nu) + \tfrac{1}{2})$$

$$= \frac{\hbar Q^2}{8\pi M_k} \int_0^\infty \frac{1}{\nu} \coth \frac{h\nu}{2kT} g(\nu) \, d\nu \qquad (20)$$

Equation (68 chapter II) gives $g(\omega)$ in the Debye approximation as $g(\omega) = \frac{9nN}{\omega_m^3}\omega^2$.

where $\omega = 2\pi\nu$

So, equation (20) in the Debye approximation can be simplified to give :

$$W_D(k) = \frac{3\hbar^2 Q^2}{2 M_k k_B \Theta} \left[\frac{1}{4} + \Lambda\left(\frac{\Theta}{T}\right)\right] \tag{21}$$

$$\text{where } \Lambda(x) = \frac{1}{x^2} \int_0^x \frac{\beta}{(e^{\beta} - 1)}\, d\beta \tag{22}$$

$\Lambda(x)$ is tabulated by Ringo (1956).

Chapter III

Lattice dynamics of cubic metals :-

The equations of motion leading to the values of the angular frequency ω as a function of the wave vector q have been discussed in chapter II. Consider a cubic crystal of identical mass M, with cube side of length a.

Consider a lattice point P with coordinates $h_1a/2$, $h_2a/2$, $h_3a/2$, h_1, h_2, h_3 are integers. The interatomic force constant $\Phi^{P}_{\alpha\beta}$ was defined to be the force on the origin atom in the α direction when the atom P moves unit distance in the β direction. The force matrix Φ^{P} is symmetric. The point P is one of a set of points demanded by the symmetry of the lattice. The force matrices of the other numbers members of the set consist of rearrangements of the same set of force constants. Denote the sets by S = 1, 2, 3 ... etc.Corresponding to the nearest neighbours, 2nd nearest, ..., etc.

It was discussed in chapter II that the angular frequencies of the 3 phonons with wave vector $\bar{q}$ are equal to the square roots of the eigenvalues of the 3x3 symmetric matrix $D_{\alpha\beta}$, which is called the dynamical matrix where it was defined to be :

$$D_{\alpha\beta} = \frac{1}{M} \sum_{l'} \Phi_{\alpha\beta}(R_{ll'})\, e^{iq.R_{ll'}} \qquad (1)$$

The elements of the force matrix $\Phi^{P}_{\alpha\beta}$ is denoted by :

$$-\Phi_{\alpha\beta} = -\begin{pmatrix}\Phi_{11} & \Phi_{12} & \Phi_{13}\\ \Phi_{21} & \Phi_{22} & \Phi_{23}\\ \Phi_{31} & \Phi_{32} & \Phi_{33}\end{pmatrix} = -\begin{pmatrix} xx & xy & xz\\ yx & yy & yz\\ zx & zy & zz\end{pmatrix}$$

$$= \begin{pmatrix}\alpha_1 & \beta_3 & \beta_2\\ \beta_3 & \alpha_2 & \beta_1\\ \beta_2 & \beta_1 & \alpha_3\end{pmatrix}$$

It can be shown that the elements of the Dynamical matrix can be given by "G.L. Squires 1962"

$$D_{ii} = \frac{8}{M}\sum_s \frac{n^s}{48}\sum_j \alpha_j^s \left\{2 - C^s_{j,i}\left[C^s_{j+1,i+1}\, C^s_{j+2,i+2} + C^s_{j+2,i+1}\, C^s_{j+1,i+2}\right]\right\} \tag{2}$$

$$D_{i,i+1} = \frac{8}{M}\sum_s \frac{n^s}{48}\sum_j \beta_j^s C^s_{j,i+2}\left[S^s_{j+1,i}\, S^s_{j+2,i+1} + S^s_{j+2,i}\, S^s_{j+1,i+1}\right] \tag{3}$$

where
$$\left.\begin{aligned} C^s_{j,i} &= \cos \pi\, a\, h^s_j q_i\\ S^s_{j,i} &= \sin \pi\, a\, h^s_j q_i \end{aligned}\right\} \tag{4}$$

where i takes values 1,2,3. Subscripts of the form i+1, i+2 whose values are greater than 3 are to be interpreted as $i - 2$, and $i - 1$ respectively. Similarly for $j+1$ & $j+2$. n^s is the number of lattice points in the set s, and q_1, q_2, q_3 are the coordinates of the lattice vector $\bar{q}$. As was also discussed in chapter II, the relations between the interatomic force constants and the elastic constants C_{11}, C_{44}, C_{12} are obtained by allowing !q! to tend to zero and comparing the matrix D with the corresponding matrix for elastic waves in a continuum.

The relations for a B.C.C. are

$$\left.\begin{aligned}
2aC_{11} &= 8 \sum_s \frac{n^s}{48} \sum_j (h_j^s)^2 \, \alpha_j^s \\
2aC_{44} &= 4 \sum_s \frac{n^s}{48} \sum_j \left[(h^s_{j+1})^2 + (h^s_{j+2})^2 \right] \alpha_j^s \\
2a(C_{12}+C_{44}) &= 16 \sum_s \frac{n^s}{48} \sum_j h^s_{j+1} \, h^s_{j+2} \, \beta_j^s
\end{aligned}\right\} \qquad (5)$$

equations (5) can hold for a F.C.C. if the left hand side is devided by 2.

I worked equations (3) & (4) up to the 8th neighbour which gives (the notation of the force constants is that used by woods at al. 1962) for B.C.C.

$$
\begin{aligned}
MD_{11} = {} & 8\alpha_1 (1 - \cos\theta_1 \cos\theta_2 \cos\theta_3) \\
& + 2\alpha_2 (1 - \cos 2\theta_1) \\
& + 2\beta_2 \{2 - (\cos 2\theta_2 + \cos 2\theta_3)\} \\
& + 4\alpha_3 \{2 - \cos 2\theta_1 (\cos 2\theta_2 + \cos 2\theta_3)\} \\
& + 2\beta_3 \{2 - 2\cos 2\theta_2 \cos 2\theta_3\} \\
& + 8\alpha_4 \{1 - \cos 3\theta_1 \cos\theta_2 \cos\theta_3\} \\
& + 8\beta_4 \{2 - \cos\theta_1 (\cos 3\theta_2 \cos\theta_3 + \cos\theta_2 \cos 3\theta_3)\} \\
& + 8\alpha_5 \{1 - \cos 2\theta_1 \cos 2\theta_2 \cos 2\theta_3\} \\
& + 2\alpha_6 \{1 - \cos 4\theta_1\} + 2\beta_6 \{2 - (\cos 4\theta_2 + \cos 4\theta_3)\} \\
& + 8\alpha_7 \{2 - \cos 3\theta_1 (\cos\theta_2 \cos 3\theta_3 + \cos 3\theta_2 \cos\theta_3)\} \\
& + 8\beta_7 \{1 - \cos\theta_1 \cos 3\theta_2 \cos 3\theta_3\} \\
& + 4\alpha_8 \{2 - \cos 4\theta_1 (\cos 2\theta_2 + \cos 2\theta_3)\} \\
& + 4\beta_8 \{2 - \cos 2\theta_1 (\cos 4\theta_3 + \cos 4\theta_2)\} \\
& + 4\gamma_8 \{2 - (\cos 4\theta_2 \cos 2\theta_3 + \cos 2\theta_2 \cos 4\theta_3)\} \\
& + \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots
\end{aligned}
$$

$$
\begin{aligned}
MD_{12} = {} & 8\beta_1 \cos\theta_3 \sin\theta_1 \sin\theta_2 \\
& + 4\gamma_3 \sin 2\theta_1 \sin 2\theta_2 \\
& + 8\gamma_4 \cos 3\theta_3 \sin\theta_1 \sin\theta_2 \\
& + 8\delta_4 \cos\theta_3 (\sin\theta_1 \sin 3\theta_2 + \sin 3\theta_1 \sin\theta_2) \\
& + 8\beta_5 \cos 2\theta_3 \sin 2\theta_1 \sin 2\theta_2 \\
& + 8\gamma_7 \cos\theta_3 \sin 3\theta_1 \sin 3\theta_2 \\
& + 8\delta_7 \cos 3\theta_3 \{\sin 3\theta_1 \sin\theta_2 + \sin\theta_1 \sin 3\theta_2\} \\
& + 8\delta_8 \sin 4\theta_1 \sin 2\theta_2 + \dots
\end{aligned}
\tag{7}
$$

where

$$
\left.
\begin{aligned}
\theta_1 &= \frac{aq_1}{2} \\
\theta_2 &= \frac{aq_2}{2} \\
\theta_3 &= \frac{aq_3}{2}
\end{aligned}
\right\}
\tag{8}
$$

From the Determinantial equation

$$
\left| D_{\alpha\beta} \binom{q}{kk'} - \omega^2 \delta_{\alpha\beta} \delta_{kk'} \right| = 0 \tag{9}
$$

which is derived as equation (15) in chapter (2), we can solve for ω^2, after now we can find the matrix elements from equations (2),(3),(4),(7),(8),(9).

The problem is facilitated by using the symmetry elements and solving along the symmetry directions. In our case for the body centred cubic, the Brillouin zone which is given in fig.(4) shows the directions, $\Delta : [00\zeta]$, $\Sigma : [\zeta\zeta 0]$, $\Lambda : [\zeta\zeta\zeta]$ which are the three major directions along which the three vibrational branches can be classified as being longitudinal or transversal.

Along the directions $D : [\frac{1}{2}\frac{1}{2}\zeta]$ and $G : [\zeta\zeta 1]$, the branches can not be classified as being longitudinal or transversal. At the high symmetry points which are :

$\Gamma(000)$, $H(001)$, and $P(\frac{1}{2}\frac{1}{2}\frac{1}{2})$, all branches are degenerate.

At the symmetry point $N(\frac{1}{2}\frac{1}{2}0)$ or its equivalent $N'(\frac{1}{2}\frac{1}{2}1)$ all branches are non-degenerate. At these symmetry points and lines, the dynamical matrix factors and the ω^2's are linear combinations of the force constants.

The results along the symmetry lines mentioned above can be summarized as :

$[00\zeta]_{\Delta}$

$M\omega_L^2 = D_{33}$ $\bar{e}_L = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$; $\bar{e}_T = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$; $\bar{e}_T = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$

$M\omega_T^2 = D_{11}$ at point H, $D_{11} = D_{33}$

$M\omega_T^2 = D_{11}$

$[\zeta\zeta 0]_{\Sigma}$

$M\omega_L^2 = D_{11}+D_{12}$

$M\omega_{T_1}^2 = D_{11}-D_{12}$ $\bar{e}_L = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}$; $\bar{e}_{T_1} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{bmatrix}$, $\bar{e}_{T_2} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$

$M\omega_{T_2}^2 = D_{33}$

$[\zeta\zeta\zeta]_{\Lambda, F}$

$M\omega_L^2 = D_{11}+2D_{12}$

$M\omega_T^2 = D_{11}-D_{12}$ $\bar{e}_L = \begin{bmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ -1/\sqrt{3} \end{bmatrix}$; $\bar{e}_T = \begin{bmatrix} 2/\sqrt{6} \\ -1/\sqrt{6} \\ -1/\sqrt{6} \end{bmatrix}$; $\bar{e}_T = \begin{bmatrix} 0 \\ 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}$

$M\omega_T^2 = D_{11} - D_{12}$ at point P, $D_{12} = 0$

$[\tfrac{1}{2}\tfrac{1}{2}\zeta]$ D

$M\omega_{\Lambda}^2 = D_{33}$ $\bar{e}_{\Lambda} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$, $\bar{e}_{\Sigma} = 1/\sqrt{2} \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}$, $\bar{e}_{\Pi} = 1//2 \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$

$M\omega_{\Sigma}^2 = D_{11}-D_{12}$

$M\omega_{\Pi}^2 = D_{11}+D_{12}$ at point P, $D_{12}=0$, threfore Σ is just the mirror image of Π across the point P.

$[\zeta\zeta 1]$ G

$$M\omega_{\Lambda}^2 = D_{11}+D_{12} \quad \bar{e}_{\Lambda} = 1/\sqrt{2}\begin{bmatrix}1\\1\\0\end{bmatrix}; \ \bar{e}_{\pi_2} = \begin{bmatrix}0\\0\\1\end{bmatrix}, \ e_{\pi_1} = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\\0\end{bmatrix}$$

$$M\omega_{\pi_2}^2 = D_{33}$$

$$M\omega_{\pi_1}^2 = D_{11} - D_{12}$$

The branches $[\zeta\zeta 0]_{T_1}$, $[\frac{1}{2}\frac{1}{2}\zeta]_{\Sigma}$ and $[\zeta\zeta 1]_{\pi_1}$ have their polarization vectors perpendicular to the mirror plane $(1\bar{1}0)$.

and since for the Bravais Lattice

$$\frac{d\sigma^{c}{}_{\pm}(q,j)}{d\Omega} \propto \left[Q.e_j(q)\right]^2 ,$$

One would not be able to observe phonons with $e_j \perp Q$ and to obtain phonons belonging to these branches one has to go to (001) plane.

Since in the symmetry directions $M\omega^2$'s are just linear combinations of the dynamical matrix elements, Lomer (1962) expressed equations (2), (3) & (9) in the form

$$M\omega_j^2 = \Phi_0 + \sum_n \Phi_n \left[1 - \cos\frac{n\pi\zeta}{\zeta_m}\right] \qquad (10)$$

where Φ_n's are called the interplaner force constants and Φ_0 is non-zero only for branches in $[\zeta\zeta 1]$ & $[\frac{1}{2}\frac{1}{2}\zeta]$ directions. where ζ is the reduced wave vecotr defined by the relation

$$\bar{q} = \frac{2\pi}{a}\zeta$$

and ζ_m is the reduced wave vector coordinate of half the distance to the nearest reciprocal lattice point so that

$$\bar{q}.\bar{R}_\ell = \frac{2\pi}{a}\,\frac{|\zeta|}{|\tau_m|} = \frac{\pi}{a}\,\frac{|\zeta|}{|\tau_m|/2} = \frac{\pi\zeta}{\zeta_m}$$

So that if we consider the nth plane from the reference atom, we will have, for atoms in that plane

$\bar{q}\cdot\bar{R}_\ell = n\pi\zeta/\zeta_m$ which defines a plane.

And since $e^{-i\bar{q}.\bar{R}_\ell}$ inters the definition of the dynamical matrix, we will at last end with equation (10). Comparing equation (10) with equations (2) & (3), we find that the interplaner force constants Φ_n are just a linear combination of individual force constants of successive neighbours. The connection between the interplanar force constants and the interatomic force constants are shown up to 8th neighbours in table (1) which is an extension of the one given by Woods et al. (1962) and Chen (1964). In terms of Φ_n, the elastic constants are given by :

$$B_i \quad a \quad c_i = \sum_n \frac{n^2}{2}\,\Phi_n \qquad (11)$$

In table (2), B_i and c_i are given for the symmetry directions in both B.C.C. & F.C.C.

Chapter IV

Experimental and Measurements :-

Measurements of the dispersion relations of lattice vibrations in Body centred cubic Iron were carried out at the NRU reactor of Chalk River (Atomic Energy of Canada Limited) using the triple axis spectrometer whose construction and operations have been published by (Mcalpin 63; Brockhouse 61). A schematic layout of the spectrometer is given in fig. (I), where :

C_1 : collimating tube of divergence 0.85°.

C_2 : collimating tube of $2\frac{1}{2}'' \times 2\frac{1}{2}'' \times 18''$ where one can put a quartz filter.

C_3 : Soller collimator of horizontal divergence 0.72°.

C_4 : Soller collimator of horizontal divergence 0.9°.

C_5 : Soller collimator of horizontal divergence 2.7°.

X_1 : Aluminium monochromating crystal (cylindrical in shape with $[1\bar{1}0]$ axis vertical with a mosaic spread of 0.65°.

X_2 : Aluminium analyzing crystal (cut with the surface nearly parallel to (111)plane) with a mosaic spread of 0.575°.

M_1 : Monitor fission counter with efficiency 1×10^{-6} counts/neutron.

M_2 : Monitor fission counter with efficiency 2×10^{-4} counts/neutron.

$B^{10}F_3$ Counter: 96% $B^{10}F_3$ enriched with active length 21.3 cm., diameter 6.2 cm.

The beam size at the sample position is 5cm x 5 cm and the estimated flux (monochromatic) of about 1×10^6 neutrons/sec.cm^2. The vertical divergence of the beam at the sample position is about 0.6° on the incident side and 1.6° on the outgoing side. So the triple axis spectrometer essentially consists of a monochromator, a specimen table and an analyzer together with a detector. The motion of three axes are independently controllable by a preprogrammed panched tape . There is another controllable degree of freedom which is the relative positions of the analyzer spectrometer with respect to the specimen (φ). The scattering angle of neutrons from the monochromator and the analyzer are $2\theta_M$ & $2\theta_A$ respectively. The relative orientation of the specimen with respect to the incoming and outgoing neutrons is specified by the angle ψ . i.e., the spectrometer is capable of feeding in monochromatic neutrons in a certain direction $\bar{K}_0$ to the specimen and then measuring both the angular and energy distributions of the scattered neutrons. To ensure that the specimen recieves a fixed number of neutrons during each counting period, a pre-set count monitor fission counter is used to start and stop the BF_3 detector.

At the time the measurements on Iron were taken, a germanium crystal was used as an analyser (the(111)plane) to get rid of the higher order reflections.

In genral to eliminate the detection of the scattered second order neutrons, the condition that $4E' > E_0 + h\nu_{max}$ is imposed in planning the experiment, where ν_{max} is the maximum frequency of the branch being measured in an energy loss experiment; there is an additional condition which is

$$E_0 - E' \leqslant h\ \nu_{max}.$$

i.e. the requirement on the $2\theta_A$ setting is $E' > \frac{3}{2}\ h\nu_{max}$. If it is required to work at higher resolution i.e. at large $2\theta_A$, this condition can be violated if a 6" quartz crystal is put in the incoming white beam to filter out the second order beam. According to the absorption coefficient vs energy curves of quartz given by (Brockhouse 61), we lose 2/3 of the primary flux. Another effective second order neutron elliminator is the pyrolitic graphite by placing it in front of the analyzer crystal.

In planning the experiment to measure a branch along certain symmetry direction, we choose a direction between the many equivalent directions in the reciprocal space so that $(Q.e)^2$ takes its maximum value. This is because the intensity is proportional to $(Q.e)^2$ (This is discussed in the last chapter on the scattering of neutrons).

Another thing is to avoid the contribution from any other mode which is perpendicular to the one we measuring e.g. if we are measuring the longitudinal mode we have to be sure that any neutron group seen comes from a longitudinal vibration. It is absolutely necessary for a successful analysis of the dispersion curves in terms of interatomic forces that the branch be correctly assigned as to character and polarization.

Another important thing to be taken into consideration on planning an experiment is the focusing effects(Brockhouse 61).

If an angular spread δ_M is introduced which allows a bundle of rays $\underline{\underline{k}}_o$ to fall on the specimen instead of a single ray, an energy spread δE_o (or δk_o) will be introduced and there will be a spread in the values of $\underline{\underline{q}}$.

If a vector diagram is drawn so that $\bar{k}_o - \bar{k}' = 2\pi\tau - \bar{q}$.,all the diagrams will be in resonance, i.e. satisfying the relations

$$Q = k_o - k' = 2\pi\tau - \bar{q}$$

$$h = E_o - E' = \pm\hbar\omega_s \text{ if}$$

$$(C_s + V_o).\delta k_o = 0 \qquad (1)$$

where

$$\underline{C}_s = \mathrm{grad}_q\, \omega_s$$

$$v_o = \frac{\hbar}{m}\; k_o$$

The condition for focusing depends on the orientation and magnitude of the gradient C_s (the group velocity) relative to v_o, i.e. relative to k_o.

If all the resolution elements contribute at once to the intensity, then as we go through the successive positions of a"constant Q" experiment we will obtain an exceedingly sharp intense line while in a defocussed configuration, a broad line with the same integrated intensity is obtained.

In equation (1), v_o will be replaced by v' when we repeat the same discussion with the analyser instead. A spread in k_o will be introduced, which is followed by a spread in $\bar{q}$, in case there is mosaic spread in the monochromating or the analyzing crystal.

In planning our constant Q experiment we always studied the transverse phonons with $\bar{q}$ in the anticlookwise sense from a reciprocal lattice point.

Measurements :

The single crystal employed was a randomly oriented cylinder of diameter 3/8 inch and length two inches which was grown by strain-anneal from Armcs iron by research Crystals Incoroporated of Richmond, virginia. The mosaic width of the crystal was 0.2°.

The measurements were carried out at room temperature. The directions along which the measurements were taken are shown in fig.(4) in the $(1\bar{1}0)$ plane of the reciprocal lattice and in fig.(5) in the (100) plane of the reciprocal lattice. These positions were chosen to obtain intense and well focused peaks as possible. The neutron groups(some of them are shown in fig.(6)) were well formed and quite intense and the centre of the peak was located accurately within the assigned errors.

The phonons were measured in the five symmetry directions Δ, Σ, Λ, D and G. Their frequencies together with their wave vectors are listed in tables (3) & (4).

All the phonons are measured in the $(1\bar{1}0)$ Mirror plane of the reciprocal lattice space except the phonons in $[\zeta\zeta 0]_{T_1}$ and $[\zeta\zeta 1]_{\pi_1}$. The $[\zeta\zeta 0]_{T_1}$ branch is measured in the (001) plane using Mcmaster University triple axis spectrometer. The measurements of the phonons along the symmetry direction

Table 3

Frequencies(in units of 10^{12}c/sec.) of phonons at room temperature measured at some specific points in the reciprocal space (chalk river).

$[\zeta 0 0]$		$[\zeta 0 0]$	
ζ	ν	ζ	ν
0.25	3.23±0.04	0.25	4.49±0.06
0.50	5.94±0.03	0.50	7.44±0.08
0.75	7.74±0.06	0.75	8.64±0.13
1.00	8.52±0.10	1.00	8.52±0.10
$[\zeta\zeta\zeta]$		$[\zeta\zeta\zeta]$	
ζ	ν	ζ	ν
0.125	2.22±0.06	0.125	4.52±0.05
0.250	4.56±0.06	0.250	7.72±0.04
0.375	6.26±0.06	0.375	8.38±0.11
0.500	7.15±0.08	0.500	7.15±0.08
0.625	7.90±0.10	0.625	5.78±0.08
0.750	8.24±0.10	0.750	6.22±0.08
0.875	8.40±0.25	0.875	7.72±0.10
1.000	8.52±0.10	1.000	8.52±0.10
$[\zeta\zeta 0]$		$[\zeta\zeta 0]$	
ζ	ν	ζ	ν
0.125	2.31±0.05	0.125	3.58±0.08
0.250	4.45±0.03	0.250	6.63±0.14
0.375	5.92±0.03	0.375	8.82±0.12
0.500	6.49±0.08	0.500	9.19±0.16
$[\frac{1}{2}\frac{1}{2}\zeta]_{\Lambda}$		$[\frac{1}{2}\frac{1}{2}\zeta]_{\pi}$	
ζ	ν	ζ	ν
0.00	6.49±0.08	0.00	4.56±0.08
0.25	6.75±0.18	0.25	5. 58±0.05
0.50	7.15±0.08	0.50	7.15±0.08
0.75	6.75±0.18	0.75	8.63±0.09
1.00	6.49±0.08		
$[\zeta\zeta 1]_{\Lambda}$		$[\zeta\zeta 1]_{\pi_2}$	
ζ	ν	ζ	ν
0.00	8.52±0.10	0.00	8.52±0.10
0.25	6.87±0.10	0.25	7.36±0.10
0.50	4.56±0.08	0.50	6.49±0.08

Table 4

Frequencies (in units of 10^{12} c/sec) of phonons at Room temperature measured at some specific points in the reciprocal space with McMaster University triple axis spectrometer.

$[\zeta\zeta 0]_{T_1}$		$[\zeta 0 0]_{T}$	
0.0625	0.80±0.03	0.125	1.66±0.06
0.1250	1.63±0.04	0.1875	2.48±0.04
0.1875	2.40±0.04	0.250	3.39±0.05
0.250	3.13±0.04		
0.375	4.20±0.05		
0.500	4.53±0.05		

$[\zeta\zeta 0]_{T_1}$ are shown in table (4) . The $[\zeta\zeta 1]_{\Pi_1}$ branch will be measured in the (001) plane of the reciprocal space with the chalk - River triple axis spectrometer. The reason is that frequencies along the $[\zeta\zeta 1]_{\Pi_1}$ are high, and since the cross-section is inversely proportional to the frequency it was not possible to measure the frequencies along the $[\zeta\zeta 1]_{\Pi_1}$ branch at McMaster because the intensity is not high enough for these frequencies. The phonon measured at $\zeta = 0.875$ in the $[\zeta\zeta\zeta]_T$ direction has contribution to the intensity from both the transverse branch and the longitudinal branch. This shifted the frequency to $\nu = 8.17 \pm 0.17$. Since the intensity is proportional to $(Q.e)^2$, it was possible to separate the contribution of the L-Branch from that of the T-Branch and found out the frequency at $\zeta = 0.875$ for the T Branch to be equal to 8.40 ± 0.25, otherwise all the phonons were well formed. So, in identifying branches through the factor $(Q.e)^2$ in the one phonon cross-section, one has to be careful. In order to observe the longitudinal phonon, one selects $\bar{Q}$ parallel to $\bar{q}$ direction as possible so that $(\bar{Q}.\bar{e})^2 = Q^2$ which gives maximum intensity. Still, this does not always ensure that we would not observe the transverse phonons. The transverse phonons of the same $\bar{q}$ can sometimes appear together with the longitudinal phonons and since the transverse phonon is usually better focused, one could misidentify the transverse phonon as the longitudinal one. The reason of occurence is due to the double scattering process

(Brockhouse 1962). These anomalous neutron groups tend to occur for a specimen with large moscaic spread.

In case one has doubt about the possible occurence of the anomalous neutron groups, one can always change to different analyser angles and repeat the measurements.

During the work on iron, the measurements were done in the constant Q mode using the(200) plane of the monochromator crystal (Aluminium). K' was kept constant. The (111) plane of the germanium analyser was used to get rid of the second order reflections.

Since this work was undertaken, a more complete set of measurements have become available by Shirane et al on the new triple axis spectrometer at Brookhaven national laboratory. We compared our results with theirs. Although measurements were not taken at identical q's in the two sets of data, it was possible to interpolate the Brookhaven results realibly to obtain frequencies at our q's . The mean ratio was found to be:

$$\left\langle \frac{\nu\,(\text{Brockhaven})}{\nu\,(\text{McMaster})} \right\rangle = 1.006.$$

The standard deviation of a single ratio from the mean was 0.014 and the standard deviation of the mean was 0.0023. This suggests that each set of measurements has an accuracy of about 1% and that there is a real determinate error in one or both of the experiments of about 0.6%.

Chapter V

Discussion

(1) The general force model of Born and Von-Kármán was formulated and discussed in chapter II & III.

(2) Central force Model (Born M. & Huang 1954).

In this model, the potential energy between two particles of the type k &k' are considered to be a function of the square of their distance apart.

If we consider $\psi(|r_{\ell\ell'}|^2)$ the potential energy between two particles a function of the square of their separation, then the total potential function of the lattice is

$$\Phi = \frac{1}{2} \sum_{\ell} \sum_{\ell'} \psi\left(|r_{\ell\ell'}|^2\right) \tag{1}$$

Let $\rho_{\ell\ell'} = |r_{\ell\ell'}|^2 = \left|\underline{R}(\ell,\ell') + \underline{u}(\ell) - \underline{u}(\ell')\right|^2$

where

$\underline{R}(\ell,\ell')$ = the equilibrium separation of the two atoms ℓ, ℓ'

$\underline{U}(\ell)$ = the displacement from equilibrium of the atom ℓ.

$\underline{U}(\ell')$ = the displacement from equilibrium of the atom ℓ'.

Again define

$$\psi' = \frac{d\psi}{d\rho} \quad , \psi'' = \frac{d^2\psi}{d\rho^2}$$

$$\therefore \quad \frac{\partial \Phi}{\partial u_\alpha(\ell'')} = \frac{1}{2} \sum_{\ell} \sum_{\ell'} \psi' \frac{\partial}{\partial u_\alpha(\ell'')} \left| R(\ell,\ell') + \underline{u}(\ell) - \underline{u}(\ell') \right|^2$$

$$= \sum_{l'} \psi' \left[R_\alpha(l'', l) + u_\alpha(l'') - u_\alpha(l') \right] - \sum_{l} \psi' \left[R_\alpha(l, l'') + u_\alpha(l) - u_\alpha(l'') \right]$$

$$= 2 \sum_{l'} \psi' R_\alpha(l'', l) + 2 u_\alpha(l'') \sum_{l'} \psi' - 2 \sum_{l'} \psi' u_\alpha(l') \qquad (2)$$

obviously $\Phi_\alpha = \left. \frac{\partial \Phi}{\partial u_\alpha(l)} \right|_{r_{l'l} = R(l', l)} = 0$

Since at equilibrium $\psi' = 0$ and all the U's at equilibrium vanish.

from equation (2) we get

$$\frac{\partial^2 \Phi}{\partial u_\beta(l''') \partial u_\alpha(l'')} = 2 \sum_{l'} R_\alpha(l'', l') \psi'' \frac{\partial \rho(l'', l')}{\partial u_\beta(l''')}$$

$$+ 2 u_\alpha(l''') \sum_{l'} \psi'' \frac{\partial \rho(l'', l')}{\partial u_\beta(l''')}$$

$$- 2 \sum_{l'} \psi'' u_\alpha(l') \frac{\partial \rho(l'', l)}{\partial u_\beta(l''')} - 2 \sum_{l'} \psi' \frac{\partial u_\alpha(l')}{\partial u_\beta(l''')}$$

$$= -4 R_\alpha(l'', l''') \psi'' \left[R_\beta(l'', l''') + u_\beta(l'') - u_\beta(l''') \right]$$
$$- 4 u_\alpha(l'') \psi'' \left[R_\beta(l'', l''') + u_\beta(l'') - u_\beta(l''') \right]$$
$$+ 4 \psi'' u_\alpha(l''') \left[R_\beta(l'', l''') + u_\beta(l'') - u_\beta(l''') \right] - 2 \psi' \frac{\partial u_\alpha(l''')}{\partial u_\beta(l''')}$$

where $\dfrac{\partial u_\alpha(l''')}{\partial u_\beta(l''')} = \delta_{\alpha\beta}$

at equilibrium all the U's are zero, thus

$$\Phi_{\alpha\beta}(\underline{R}(l'l)) = \frac{\partial^2 \Phi}{\partial u_\alpha(l)\,\partial u_\beta(l')}\bigg|_{R(l'l)}$$

$$= \left[-2\psi'\delta_{\alpha\beta} - 4R_\alpha(l,l')R_\beta(l,l')\psi''\right]_{R_{ll'}}$$

or

$$\Phi_{\alpha\beta}(\underline{R}_{ll'}) = \left[-2\psi'\delta_{\alpha\beta} - 4R_\alpha(l,l')R_\beta(l,l')\psi''\right]_{\underline{R}_{ll'}}$$

where we have previously defined

$-\Phi_{\alpha\beta}(l,l')$ as the force on atom l in the α direction when atom l' is moved a unit distance in the β direction.

Let us work out the central force Model for the Body centred cubic.

The matrix elements for the force constants as defined in chapter III is :

$$-\Phi_{\alpha\beta} = \begin{pmatrix} xx & xy & xz \\ yx & yy & yz \\ zx & zy & zz \end{pmatrix}$$

The 1st mearest neighbour to the atom at the origin is the set of atoms $\frac{a}{2}$ (111) which has a force constant matrix

$$-\Phi_{\alpha\beta}\left(\tfrac{a}{2}(111)\right) = \begin{pmatrix} \alpha_1 & \beta_1 & \beta_1 \\ \beta_1 & \alpha_1 & \beta_1 \\ \beta_1 & \beta_1 & \alpha_1 \end{pmatrix}$$

$$= 2\psi'\delta_{\alpha\beta} + 4R_\alpha(\ell,\ell')R_\beta(\ell,\ell')\psi''$$

by equation (3)

which gives $\alpha_1 = 2\psi' + a^2\psi''$

$\beta_1 = a^2\psi''$

$$\therefore \psi' = \frac{1}{2}(\alpha_1 - \beta_1) \qquad (4)$$

Similarly, for the 2nd neighbour which is the set of atoms at $\frac{a}{2}$ (200), we have :

$$\psi' = \frac{1}{2}\beta_2 \qquad (5)$$

for the third negibour, the set of atoms at $\left\{\frac{a}{2}(220)\right\}$

$$-\Phi_{\alpha\beta}\left\{\frac{a}{2}(220)\right\} = \begin{pmatrix} \alpha_3 & \gamma_3 & 0 \\ \gamma_3 & \alpha_3 & 0 \\ 0 & 0 & \beta_3 \end{pmatrix}$$

$$= 2\psi'\delta_{\alpha\beta} + 4R_\alpha R_\beta\psi''\Big|_{\text{at equilibrium}}$$

$$\therefore \alpha_3 = 2\psi' + 4a^2\psi''$$

$\beta_3 = 2\psi', \gamma_3 = 4a^2\psi''$

$$\therefore \psi' = \tfrac{1}{2}(\alpha_3 - \gamma_3) \qquad (6)$$

and

$$\alpha_3 - \beta_3 - \gamma_3 = 0 \qquad (7)$$

similarly for the 4th neighbour, the set of atoms at $\frac{a}{2}(311)$, we get :

$$\psi' = \tfrac{1}{2}(\beta_4 - \gamma_4) \qquad (8)$$

and also :

$$\left.\begin{array}{l} \delta_4 - 3\gamma_4 = 0 \\ \alpha_4 - \beta_4 - 8\gamma_4 = 0 \end{array}\right\} \qquad (9)$$

for the 5th negibour $\{a/2(222)\}$

$$\psi' = \tfrac{1}{2}(\alpha_5 - \beta_5) \qquad (10)$$

for the 6th negibour $\{a/2(400)\}$, we get

$$\psi' = \tfrac{1}{2}\beta_6 \qquad (11)$$

For the 7th neighbour (a/2(331))

$$\psi' = \tfrac{1}{2}(\alpha_7 - \delta_7) \qquad (12)$$

and also

$$\left.\begin{aligned} 3\alpha_7 - \delta_7 &= 0 \\ 3\alpha_7 - 3\beta_7 + \gamma_7 - 3\delta_7 &= 0 \end{aligned}\right\} \qquad (13)$$

For the 8th neighbour :

$$\psi' = \frac{1}{2}(\alpha_8 - 2\delta_8) \qquad (14)$$

and also

$$\left.\begin{aligned} \alpha_8 - \gamma_8 - 2\delta_8 &= 0 \\ 2\beta_8 - 2\gamma_8 - \delta_8 &= 0 \end{aligned}\right\} \qquad (15)$$

Imposing the conditions (7), (9), (13) and (15) which are now

$$\left.\begin{aligned} \alpha_3 - \beta_3 - \gamma_3 &= 0 \\ \delta_4 - 3\gamma_4 &= 0 \\ \alpha_4 - \beta_4 - 8\gamma_4 &= 0 \\ 3\gamma_7 - \delta_7 &= 0 \\ \alpha_8 - \gamma_8 - 2\delta_8 &= 0 \\ 2\beta_8 - 2\gamma_8 - \delta_8 &= 0 \end{aligned}\right\} \qquad (16)$$

gives what is called the axially symmetric model (Lehman, et al.) This means that the interaction potential is different for every set of neighbours from the others. i.e. the potential through which the 1st nearest neighbour interact with the atom at the atom at origin is not the same potential through which the <u>2nd</u> nearest neighbour interact with the atom at the centre and so on.

To have the same potential for all neighbours another condition, the stability condition, has to be imposed which is (Max Born and Huang):

$$\frac{d\psi}{d\,a} = \sum_j z_j \left(\frac{d\psi_j}{d\rho^2}\right) \frac{d\,\rho^2}{d\,a} = 0 \qquad (17)$$

Condition (17) together with conditions (16) gives the central Force Model.

To explain what equation (17) means, for example: the <u>1st</u> nearest neighbours are the 8 atoms at $\frac{a}{2}$ (111)

$\therefore$ $z_j = 8$, $\frac{d\psi_j}{d\rho^2} = \frac{1}{2}(\alpha_1 - \beta_1)$ as given by equation (4) above and

$$\rho = \frac{a}{2}\sqrt{(1)^2 + (1)^2 + (1)^2} = \frac{\sqrt{3}\,a}{2}$$

$$\therefore \quad \rho^2 = \frac{3\,a^2}{4}$$

$$\therefore \quad \frac{d\rho^2}{da} = \frac{3}{2}\,a$$

$\therefore$ for the <u>1st</u> nearest neighbour:

$$\frac{d\psi}{da} = 8 \times \frac{\alpha_1 - \beta_1}{2} \times \frac{3}{2}\,a$$

$$= 6a\,(\alpha_1 - \beta_1) \qquad (18)$$

similarly for the 2nd nearest neighbour

$$\frac{d\psi}{da} = 6\beta_2 a \qquad (19)$$

working $\frac{d\psi}{da}$ for the (1st, 2nd, 3rd, ... up to the 8th negibour) and summing over them, this gives the stability condition for the 1st 8 neighbours as :

$$\alpha_1 - \beta_1 + \beta_2 + 4\beta_3 + 11\beta_4 - 11\gamma_4$$
$$+ 4\alpha_5 - 4\beta_5 + 4\beta_6 + 19\alpha_7 - 19\delta_7$$
$$+ 20\gamma_8 = 0 \qquad (20)$$

The stability condition as given by equation (20) combined with the equation relating the atomic force constants to the elastic constants which was discussed in chapter III as B_i a $C_i = \sum_n \frac{n^2}{2} \Phi_n$ (equation 11 chapter III) Leads to the relation

$$C_{12} = C_{44} \qquad (21)$$

which is called the cauchy relation, but investigation of the experimentally measured elastic constants of metals shows that equation (21) is not satisfied in general which means that forces between ions in metals have noncentral components. The only metal until now which proved such evidence is sodium "Woods et al. 1962.".

Now: For iron, the frequencies are plotted against the component of the reduced wave vector ζ as defined in the first two chapters. A Born-Von Kármán general force model was calculated from the data for forces extending as far as 8th neighbours. It was necessary to include forces out to third neighbours; therefore only small improvements in fit were found. Force constants settled down to final values only when forces up to fifth neighbours were included. The results for the 5th neighbour force model are plotted as broken lines in fig.(3). This model can be seen to fit the data quite sufficiently within the error. The values of the force constants for this model are given in table (5) in units of 10^4 dynes/cm.

Least squares fits were also carried out after imposing the axially symmetric conditions given by equation 16 which is up to the 8th neighbours

$$\alpha_3 - \beta_3 - \gamma_3 = 0$$

$$\delta_4 - 3\gamma_4 = 0$$

$$\alpha_4 - \beta_4 - 8\gamma_4 = 0$$

$$3\gamma_7 - \delta_7 = 0$$

$$\alpha_8 - \gamma_8 - 2\delta_8 = 0$$

$$2\beta_8 - 2\gamma_8 - \delta_8 = 0$$

The values of force constants calculated under the assumptions

Table (5)

Born von-Karman 5th neighbour general force constants

a/2(111)		a/2(200)		a/2(220)		
α_1	β_1	α_2	β_2	α_3	β_3	γ_3
(xx)	(xy)	(xx)	(yy)	(xx)	(zz)	(xy)
1.628	1.507±.05	1.552±.10	0.054±.007	.118	-.088	.127

a/2(311)				a/2(222)	
α_4	β_4	γ_4	δ_4	α_5	β_5
(xx)	(yy)	(yz)	(xz)	(xx)	(xy)
-.023	.024	.039±.03	.007±.02	-.046	-.03±.05

unless given, the estimated error, in the above force constants is about ±0.025 x 10^4 dynes/cm.

Table (6)

Force constants calculated from the A-S Model

a/2(111)		a/2(200)		a/2(220)		
α_1	β_1	α_2	β_2	α_3	β_3	γ_3
(xx)	(xy)	(xx)	(yy)	(xx)	(zz)	(xy)
1.594	1.464±.026	1.547±.053	.079±.034	.090	-0.076	0.165

a/2(311)				a/2(222)	
α_4	β_4	γ_4	δ_4	α_5	β_5
(xx)	(yy)	(yz)	(xz)	(xx)	(xy)
.007	.028	-.003±.002	-.008±.007	-.032	-.003±.019

unless given, the estimated error in the above force constants is about ± 0.025 x 10^4 dynes/cm.

of this model did not change significantly within the limits of error from those calculated by the general force model as shown in table (6).

To be specific, only the force constants for 3rd and higher neighbours are different from those calculated on the basis of a general force model but they are small. If we go as far as the 8th neighbour in case of A.S. Model, we find that the fit is about equally good as that for general forces to fifth neighbours. This means that the iron force system could possibly be described by an axial symmetric model. After imposing the stability condition (20) which is :

$$\alpha_1 - \beta_1 + \beta_2 + 4\beta_3 + 11\beta_4 - 11\gamma_4 + 4\alpha_5 - 4\beta_5 + 4\beta_6 + 19\alpha_7 - 19\delta_7 + 20\gamma_8 = 0 \qquad (20)$$

it was found that with the central force model there is a significant change in the values of the calculated force constants from those calculated for a general force model and which gives a fit to the data. In table (7), the force constants for a central force model are shown for 5th neighbours. It was previously mentioned that, a condition for the validity of the central force conditions is the cauchy relation $C_{12} = C_{44}$. For Iron C_{12} & C_{44} differ by 13% according to values given by (Rayne and chandrasekhur). Previous measurements taken by G.C. Low

Table (7)

Force constants calculated from the C.F. Model

a/2(111)		a/2(200)		a/2(220)		
α_1	β_1	α_2	β_2	α_3	β_3	γ_3
(xx)	(xy)	(xx)	(yy)	(xx)	(zz)	(xy)
1.622±.02	1.462±.02	1.541±.05	.098±.03	.078±.01	-.074±.02	.153±.02

a/2(311)				a/2(222)	
α_4	β_4	γ_4	δ_4	α_5	β_5
(xx)	(yy)	(yz)	(xz)	(xx)	(xy)
-0.016±.01	.019±.01	-.004±.001	-.013±.004	-.043±.01	.01±.009

(1962) did not cover all the symmetry directions. For modes where the two sets of data overlap, the results are in reasonably good agreement with these of low within the larger errors(6%) of his measurements.

A third neighbour model calculated by him from his data differs appreciably from the corresponding model based on our data. The most important difference is in the relative sizes of the 1st neighbour force constants, In Low's Model $\beta_1(1\,x\,Y) > \alpha_1(1xx)$ which indicates the existence of a repulsive force between first neighbours, while our model gives a fit to the data based on the fact that $\alpha_1(1xx) > \beta_1(1XY)$. The fact that $\alpha_1(1xx) > \beta_1(1xy)$ indicates that the first neighbour forces are attractive which is a remarkable fact found true for all the B.C.C. transition metals so far investigated: e.g. tungsten, Niobium, Molybdenum and tantalum.

It was found that $1xx < 1xy$, i.e., a repulsive force exists between 1st neighbours as intuitively expected, for all non-transition B.C.C. metals like sodium, potessium and β Brass. This was also true, i.e. the force between 1st neighbours is repulsive, for face centred cubic metals studied so far, e.g.; Al, Pb, Pb alloys, Cu, Ni and Ni-Fe alloys.

Also the frequency distribution function $g(\nu)$ at room temperature was calculated following the method of Gilat and Raubenheimer, using the force constants obtained from the best fit (5th neighbours) . The frequency distribution curve is shown in fig.(7) which has shown pronounced peaks at $\nu = 5.7 \times 10^{12}$ c/sec, $\nu = 6.5 \times 10^{12}$ c/sec. and at $\nu = 8.625 \times 10^{12}$ c/sec. Using the computer program of Svenson et al, the Debye temperature as a function of temperature was calculated from this frequency distribution function $g(\nu)$. It can be seen from fig.(8) that it has a zero temperature value $\Theta_0(T) = 463.5$°K which is to be compared with $\Theta_0(T) = 462$°K obtained from specific heat data by Keesom & Kurrelmeyer.

Table (1)

	$\frac{a}{2}(111)$		$\frac{a}{2}(2000)$		$\frac{a}{2}(220)$			$\frac{a}{2}(311)$				$\frac{a}{2}(222)$		$\frac{a}{2}(400)$		$\frac{a}{2}(331)$				$\frac{a}{2}(420)$			
	1xx	1xy	2xx	2yy	3xx	3zz	3xy	4xx	4yy	4yz	4xz	5xx	5xy	6xx	6yy	7xx	7zz	7yz	7xy	8xx	8yy	8zz	8xy
A1	8	0	0	0	0	0	0	8	8	0	0	0	0	0	0	8	0	0	0	0	0	0	0
A2	0	0	0	2	4	4	0	0	0	0	0	8	0	0	0	0	0	0	0	4	0	4	0
A3	0	0	0	0	0	0	0	0	8	0	0	0	0	0	0	8	8	0	0	0	0	0	0
A4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	4	4	0
B1	8	0	0	0	0	0	0	0	16	0	0	0	0	0	0	0	8	0	0	0	0	0	0
B2	0	0	2	0	8	0	0	0	0	0	0	8	0	0	0	0	0	0	0	0	8	0	0
B3	0	0	0	0	0	0	0	8	0	0	0	0	0	0	0	16	0	0	0	0	0	0	0
B4	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	8	0	0	0
C1	6	2	0	0	0	0	0	2	4	-2	4	0	0	0	0	8	4	0	4	0	0	0	0
C2	0	0	2	4	0	0	0	0	0	0	0	6	2	0	0	0	0	0	0	4	4	4	4
C3	2	-2	0	0	0	0	0	4	8	4	0	0	0	0	0	0	0	0	0	0	0	0	0
C4	0	0	0	0	4	2	-2	0	0	0	0	0	0	2	4	0	0	0	0	0	0	0	0
C5	0	0	0	0	0	0	0	2	4	-2	-4	0	0	0	0	4	2	4	-2	0	0	0	0
C6	0	0	0	0	0	0	0	0	0	0	0	2	-2	0	0	0	0	0	0	4	4	4	-4
C7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	2	-4	-2	0	0	0	0
D1	6	-4	0	0	0	0	0	2	4	4	-8	0	0	0	0	8	4	0	-8	0	0	0	0
D2	0	0	2	4	0	0	0	0	0	0	0	6	-4	0	0	0	0	0	0	4	4	4	-8
D3	2	4	0	0	0	0	0	4	8	-8	0	0	0	0	0	0	0	0	0	0	0	0	0
D4	0	0	0	0	4	2	4	0	0	0	0	0	0	2	4	0	0	0	0	0	0	0	0
D5	0	0	0	0	0	0	0	2	4	4	8	0	0	0	0	4	2	-8	4	0	0	0	0
D6	0	0	0	0	0	0	0	0	0	0	0	2	4	0	0	0	0	0	0	4	4	4	8
D7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	2	8	4	0	0	0	0
E1	4	0	0	4	8	0	0	4	8	0	0	0	0	0	0	8	0	0	0	8	0	4	0
E2	0	0	0	0	0	2	0	0	8	0	0	4	0	0	4	8	0	0	0	0	0	0	0
E3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	0	0	4	0
F1	4	-4	2	2	4	4	0	4	8	-4	8	0	0	0	0	4	4	8	0	2	6	4	4
F2	0	0	0	0	2	0	-2	4	4	0	-8	4	-4	2	2	4	4	-8	0	4	0	4	0
F3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	-4	2	2	0	-4
G1	4	4	2	2	4	4	0	4	8	4	-8	0	0	0	0	4	4	-8	0	2	6	4	-4
G2	0	0	0	0	2	0	2	4	4	0	8	4	4	2	2	4	4	8	0	4	0	4	0
G3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4	0	0	4	2	2	0	4
OH	8	0	0	8	16	0	0	8	16	0	0	0	0	0	0	16	8	0	0	16	0	16	0
H1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H2	0	0	2	0	-8	0	0	0	0	0	0	8	0	0	0	0	0	0	0	0	8	0	0
H3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
H4	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	-8	0	0	0
O1	8	8	4	4	8	8	0	8	16	8	-16	0	0	0	0	16	8	-16	8	8	16	8	0
I1	0	-8	0	0	0	0	0	0	0	0	16	0	0	0	0	0	0	0	-8	0	0	0	0
I2	0	0	0	2	-4	-4	0	0	0	0	0	8	0	0	0	0	0	0	0	4	0	4	0
I3	0	0	0	0	0	0	0	0	0	-8	0	0	0	0	0	0	0	16	0	0	0	0	0
I4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	-4	-4	0
OJ	16	0	0	0	0	0	0	16	32	0	0	0	0	0	0	32	16	0	0	0	0	0	0
J1	-4	-4	2	2	4	4	0	-4	-8	-4	8	0	0	0	0	-4	-4	8	0	2	6	4	-4

Table 1. cont.

J2	0	0	0	0	2	0	2	-4	-4	0	-8	4	4	2	2	-4	-4	-8	0	4	0	4	0
J3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-4	0	0	-4	2	2	0	4
OK	16	0	0	0	0	0	0	16	32	0	0	0	0	0	0	32	16	0	0	0	0	0	0
K1	-4	0	0	4	8	0	0	-4	-8	0	0	0	0	0	0	-8	0	0	0	8	0	4	0
K2	0	0	0	0	0	2	0	0	-8	0	0	4	0	0	4	-8	0	0	0	0	8	0	0
K3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-4	0	0	0	0	4	0
OL	16	0	0	0	0	0	0	16	32	0	0	0	0	0	0	32	16	0	0	0	0	0	0
L1	-4	4	2	2	4	4	0	-4	-8	4	-8	0	0	0	0	-4	-4	-8	0	2	6	4	4
L2	0	0	0	0	2	0	-2	-4	-4	0	8	4	-4	2	2	-4	-4	8	0	4	0	4	0
L3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-4	0	0	4	2	2	0	-4
11	2	0	2	0	8	0	0	18	4	0	0	8	0	8	0	36	2	0	0	32	8	0	0
44	2	0	0	2	4	4	0	2	20	0	0	8	0	0	8	20	18	0	0	4	16	20	0
12	-2	4	0	-2	-4	-4	8	-2	-20	4	24	-8	16	0	-8	-20	-18	24	36	-4	-16	-20	32

Table (1) gives the interatomic force constant composition of interplanar force constants Φ_n and the elastic constants for symmetry branches in a body centred cubic crystal

where $M\omega^2 = \Phi_0 + \sum_n \Phi_n \left(1 - \cos \frac{n\pi\zeta}{\zeta_{max}}\right)$

The definition of the symmetry directions given in the table are :

$A = [00\zeta]_T$, $B = [00\zeta]_L$, $C = [\zeta\zeta\zeta]_T$, $D = [\zeta\zeta\zeta]_L$,

$E = [\zeta\zeta 0]_{T_2}$, $F = [\zeta\zeta 0]_{T_1}$, $G = [\zeta\zeta 0]_L$,

D_{LL} $H = [\frac{1}{2}\frac{1}{2}\zeta]_\Lambda$, Dp; $I = [\frac{1}{2}\frac{1}{2}\zeta]_\Pi$, $J = [\zeta\zeta 1]_\lambda$

$K = [\zeta\zeta 1]_{\Pi_2}$, $L = [\zeta\zeta 1]_{\Pi_1}$

where

$$\zeta_m = \begin{cases} 1 & \text{for } [00\zeta], [\zeta\zeta\zeta], [\frac{1}{2}\frac{1}{2}\zeta] \\ 0.5 & \text{for } [\zeta\zeta 0], [\zeta\zeta 1] \end{cases}$$

and the elastic constants are

$11 = ac_{11}$, $44 = ac_{44}$, $12 = ac_{12}$ where a is the lattice constant and c_{ij} are the elastic constants.

The relation between the elastic constants and the interplanar force constants are :

$$B_i a c_i = \sum_{n=1}^{N} \frac{n^2}{2} \Phi_n$$

where $B_i = 2\alpha^2 \zeta_m^2$ for B.c.c.

$= \alpha^2 \zeta_m^2$ for f.c.c. and $|\zeta| = \alpha\zeta$.

$c_i = \rho V_i^2$

and table (2) gives values for B_i and the combination of c_i

Table (2)

Branch	$\rho V_i^2 = c_i$	B_i	
		B.c.c.	F.c.c.
$[00\zeta]_T$	c_{44}	2	1
$[00\zeta]_L$	c_{11}	2	1
$[\zeta\zeta\zeta]_T$	$1/3(c_{11} - c_{12} + c_{44})$	6	3/4
$[\zeta\zeta\zeta]_L$	$1/3(c_{11} + 2c_{12} + 4c_{44})$	6	3/4
$[\zeta\zeta 0]_{T_1}$	$1/2(c_{11} - c_{12})$	1	2
$[\zeta\zeta 0]_{T_2}$	c_{44}	1	2
$[\zeta\zeta 0]_L$	$1/2(c_{11} + c_{12} + 2c_{44})$	1	2

A.E.C.L. Ref. # A-2597-G

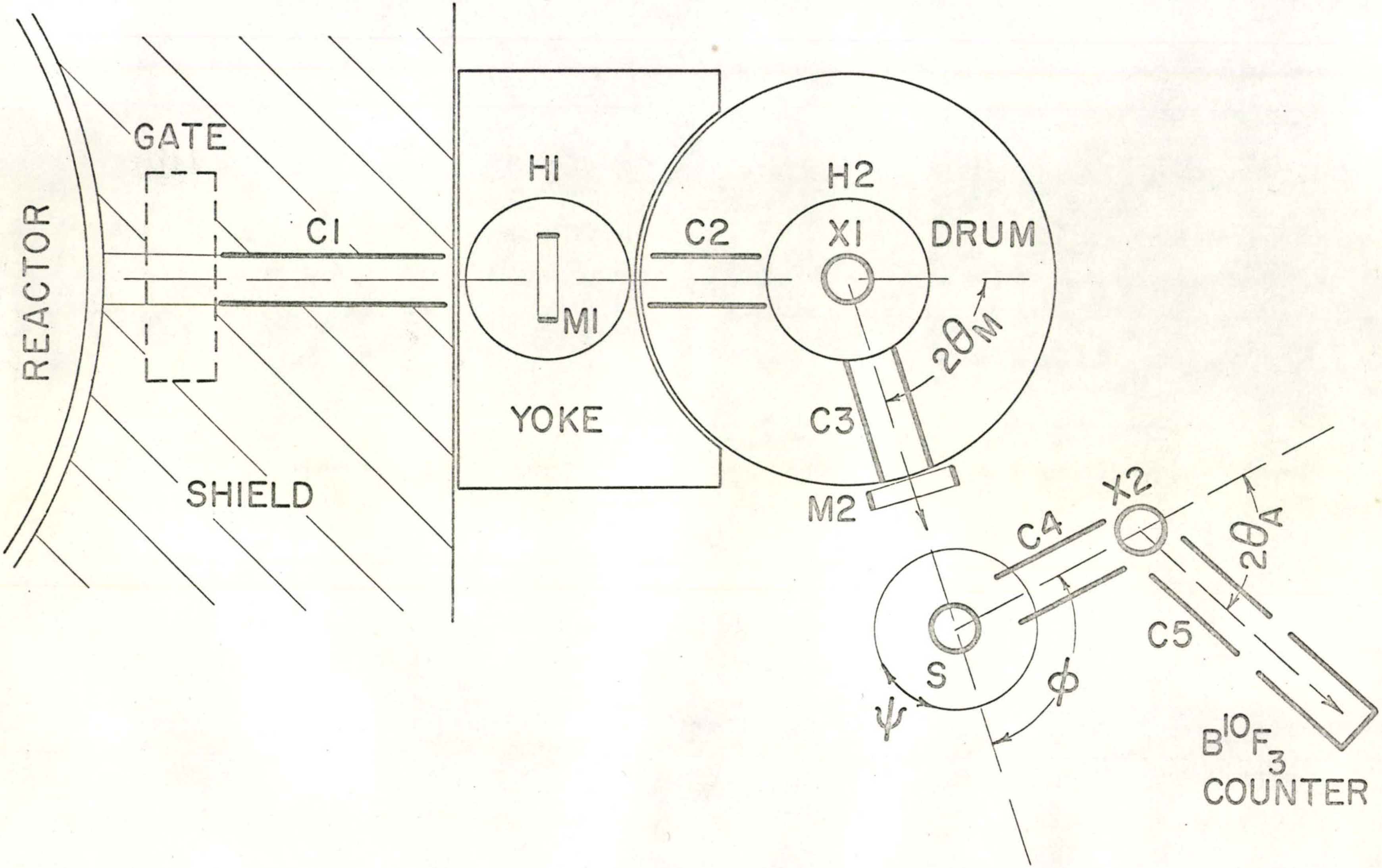
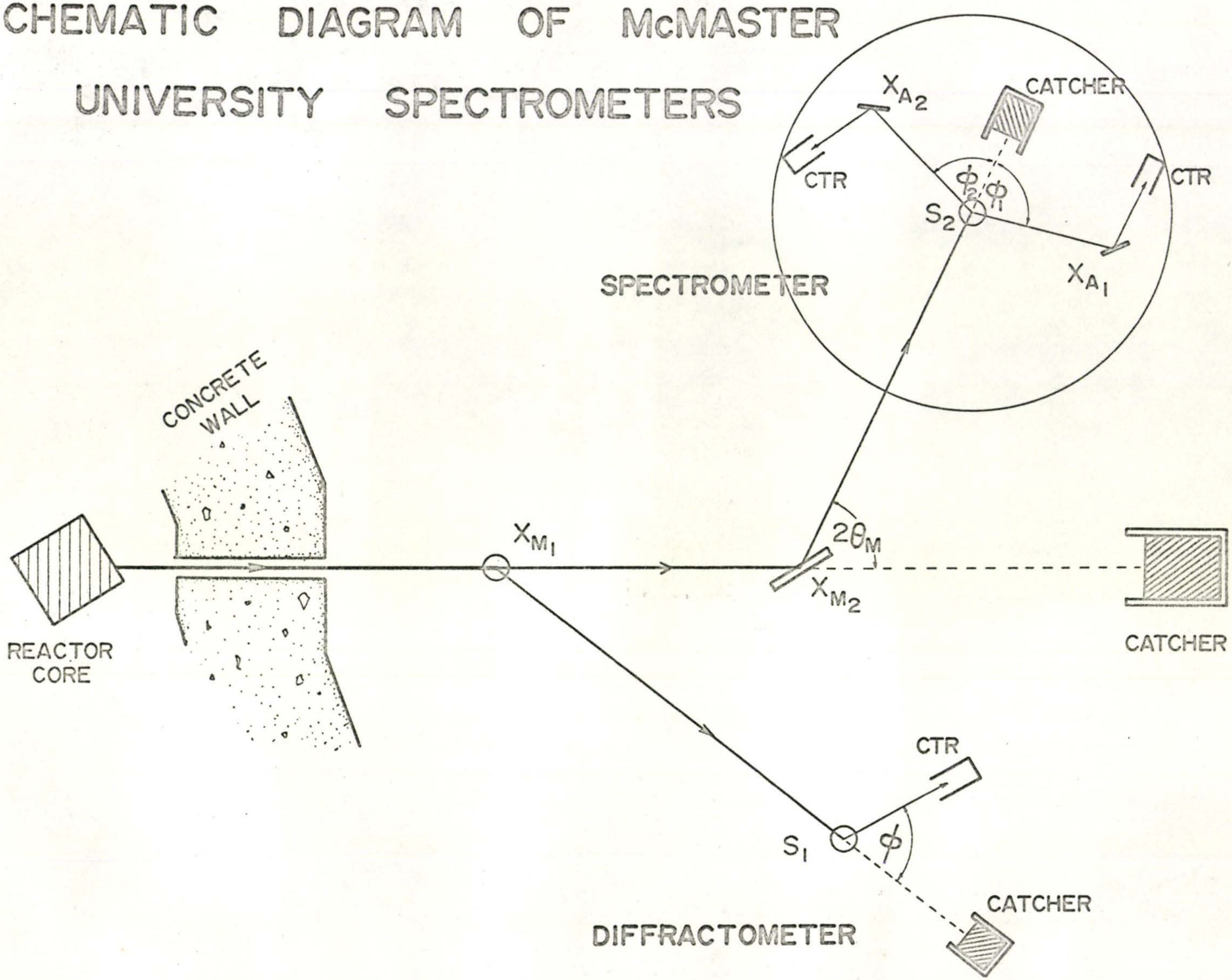


Fig.(1)

SCHEMATIC DIAGRAM OF McMASTER UNIVERSITY SPECTROMETERS



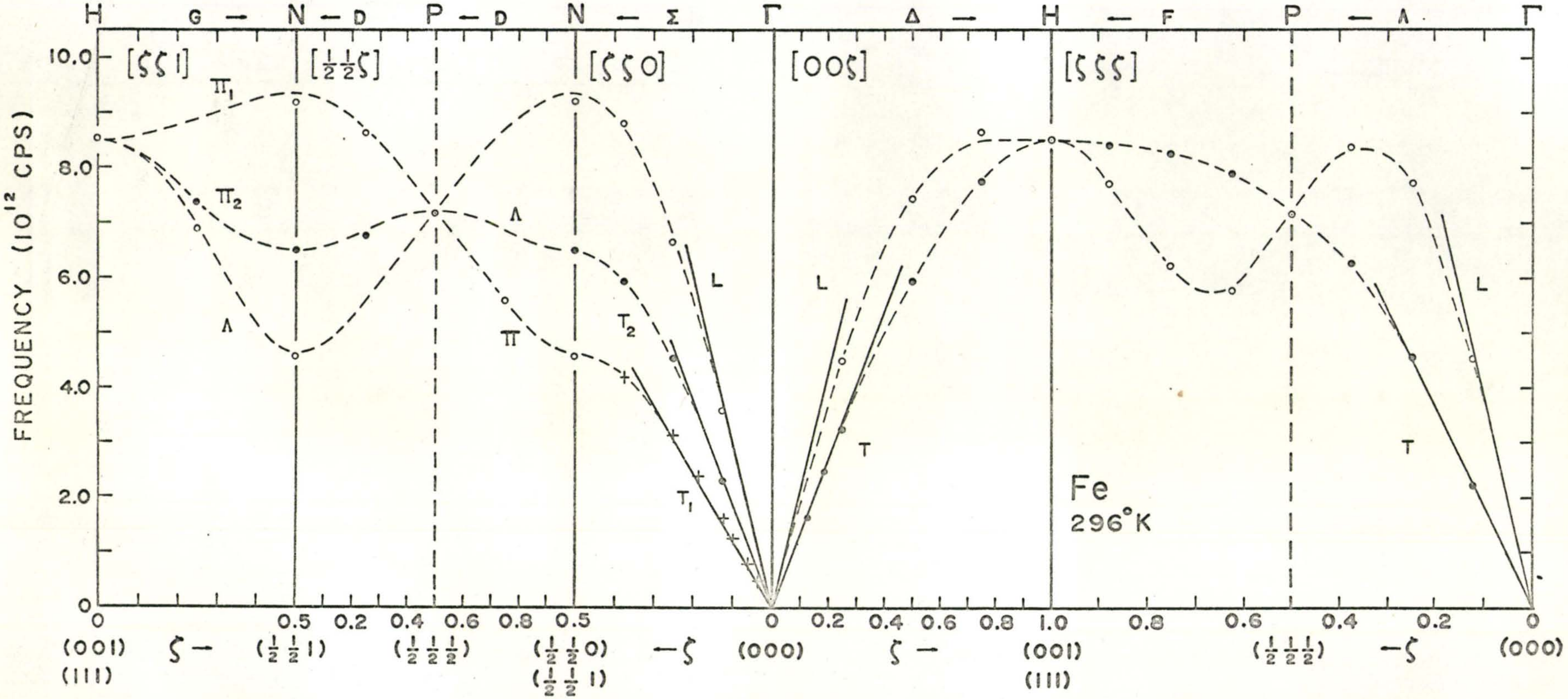
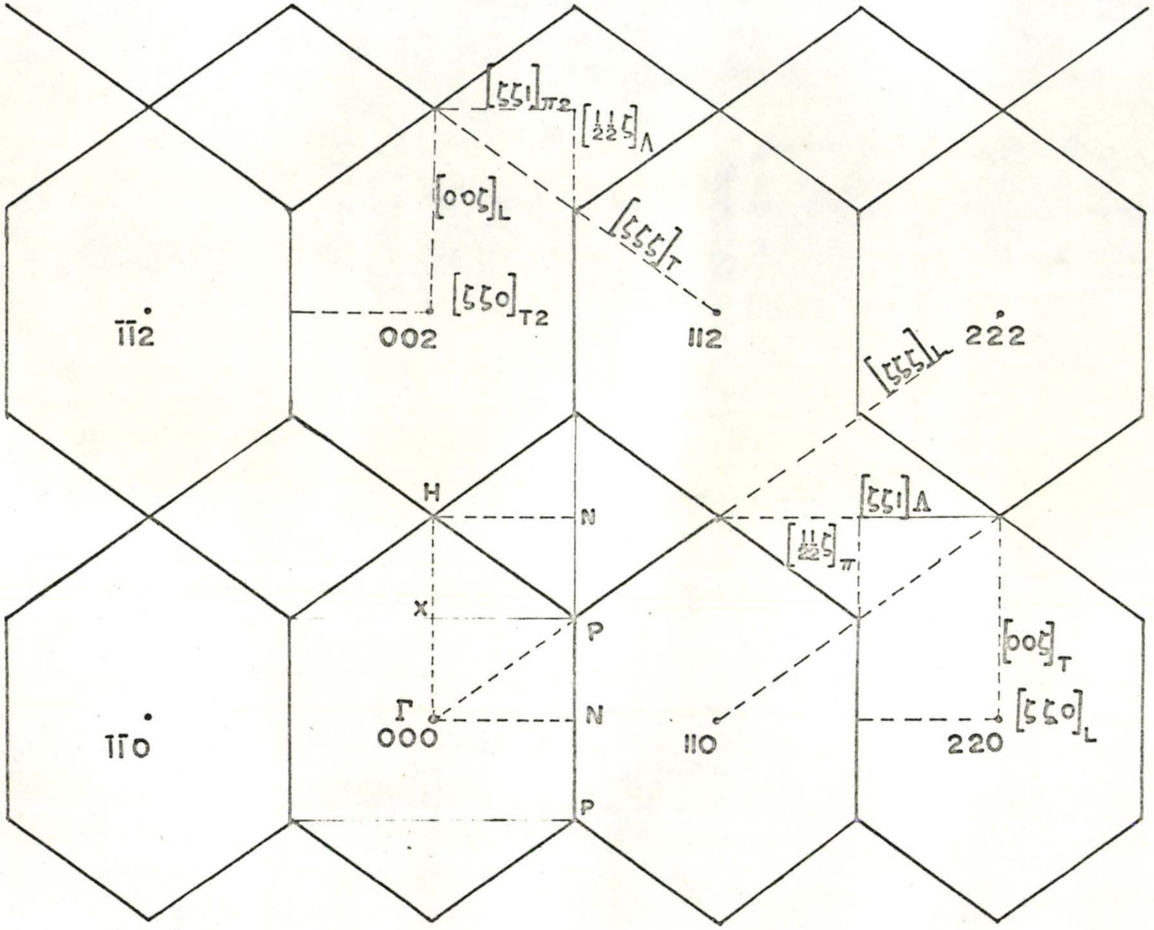

H
G →
N
← D
P
← D
N
← Σ
Γ
Δ →
H
← F
P
← Λ
Γ
[ζζ1]
[½½ζ]
[ζζ0]
[00ζ]
[ζζζ]
FREQUENCY (10¹² CPS)
10.0
8.0
6.0
4.0
2.0
0
π₁
π₂
Λ
Λ
π
T₂
T₁
L
L
T
T
L
Fe
296°K
0
0.5
0.2
0.4
0.6
0.8
0.5
0
0.2
0.4
0.6
0.8
1.0
0.8
0.6
0.4
0.2
0
(001)
(111)
ζ →
(½ ½ 1)
(½ ½ ½)
(½ ½ 0)
(½ ½ 1)
← ζ
(000)
ζ →
(001)
(111)
(½ ½ ½)
← ζ
(000)

Fig. 5 3

(1$\bar{1}$0) PLANE B.C.C. (R.L.)



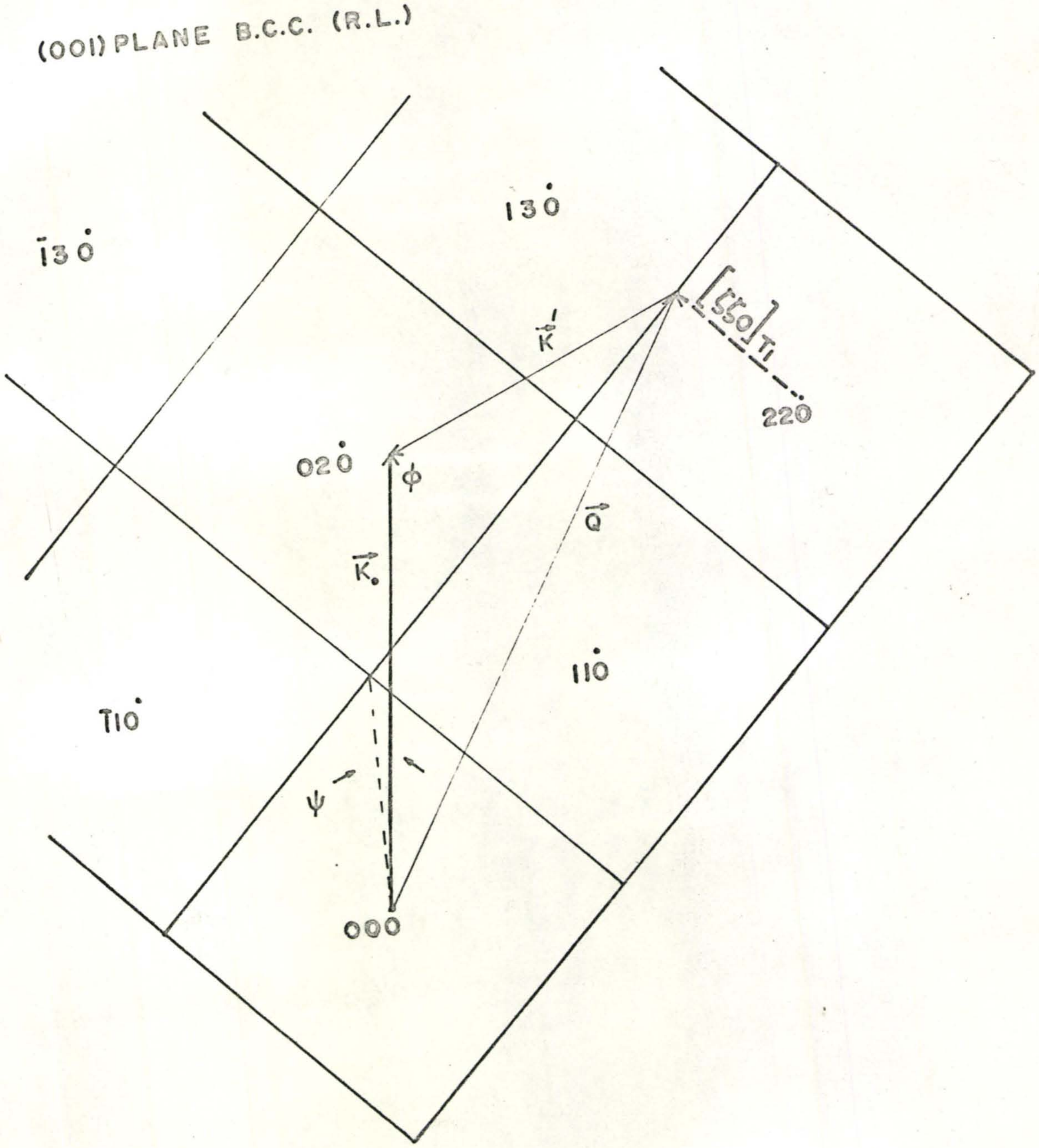

(001) PLANE B.C.C. (R.L.)
$\bar{1}30$
130
$[550]_{Ti}$
$\vec{K'}$
220
020
ϕ
$\vec{Q}$
$\vec{K_0}$
110
$\bar{1}10$
ψ
000

FIG. 5

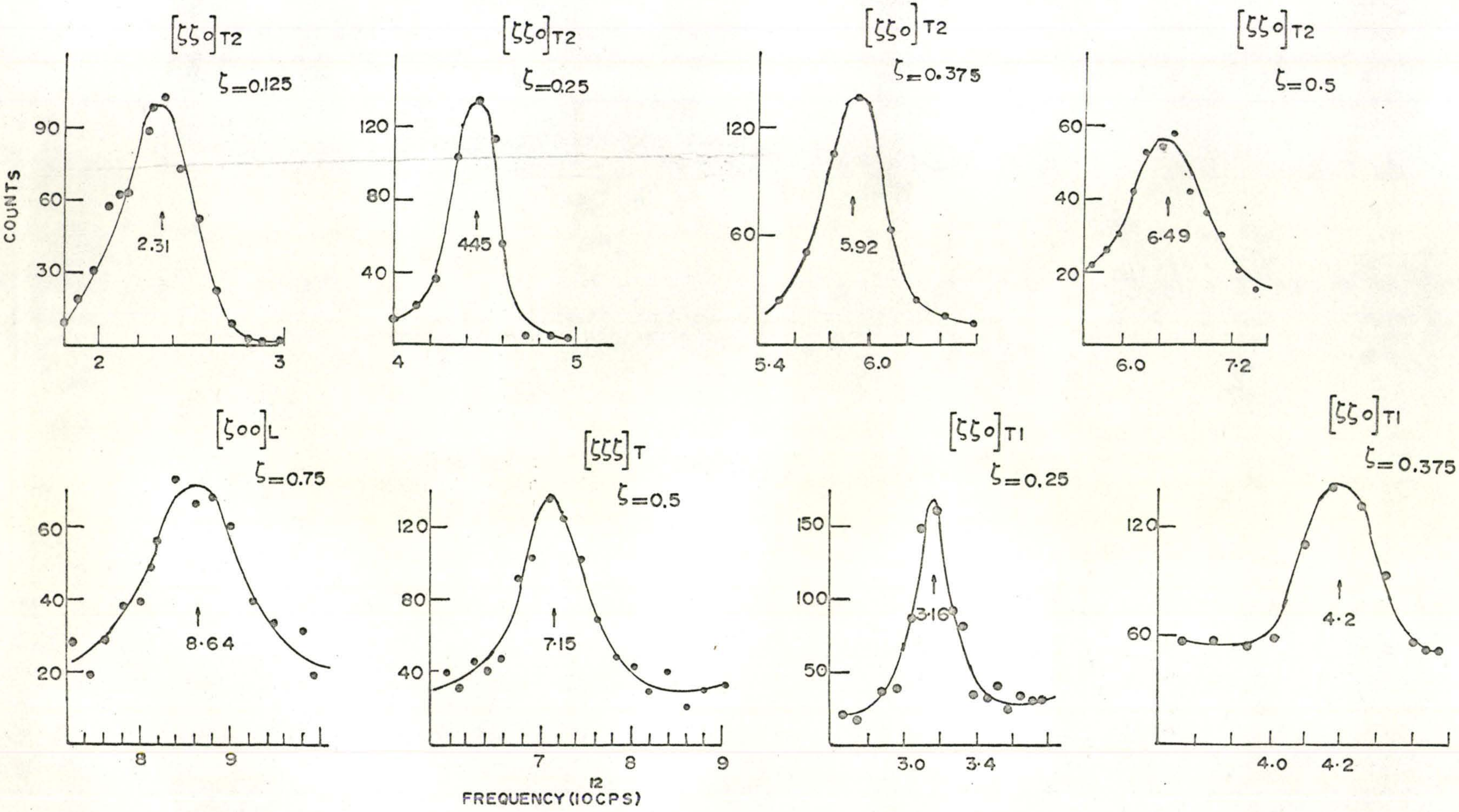

[ζζ0]T2
ζ=0.125
90
60
30
COUNTS
2.31
2
3
[ζζ0]T2
ζ=0.25
120
80
40
445
4
5
[ζζ0]T2
ζ=0.375
120
60
5.92
5·4
6.0
[ζζ0]T2
ζ=0.5
60
40
20
6·49
6.0
7·2
[ζ00]L
ζ=0.75
60
40
20
8·64
8
9
[ζζζ]T
ζ=0.5
120
80
40
7·15
7
8
9
FREQUENCY (10^12 CPS)
[ζζ0]T1
ζ=0.25
150
100
50
3·16
3·0
3·4
[ζζ0]T1
ζ=0.375
120
60
4·2
4·0
4·2

Fig.6

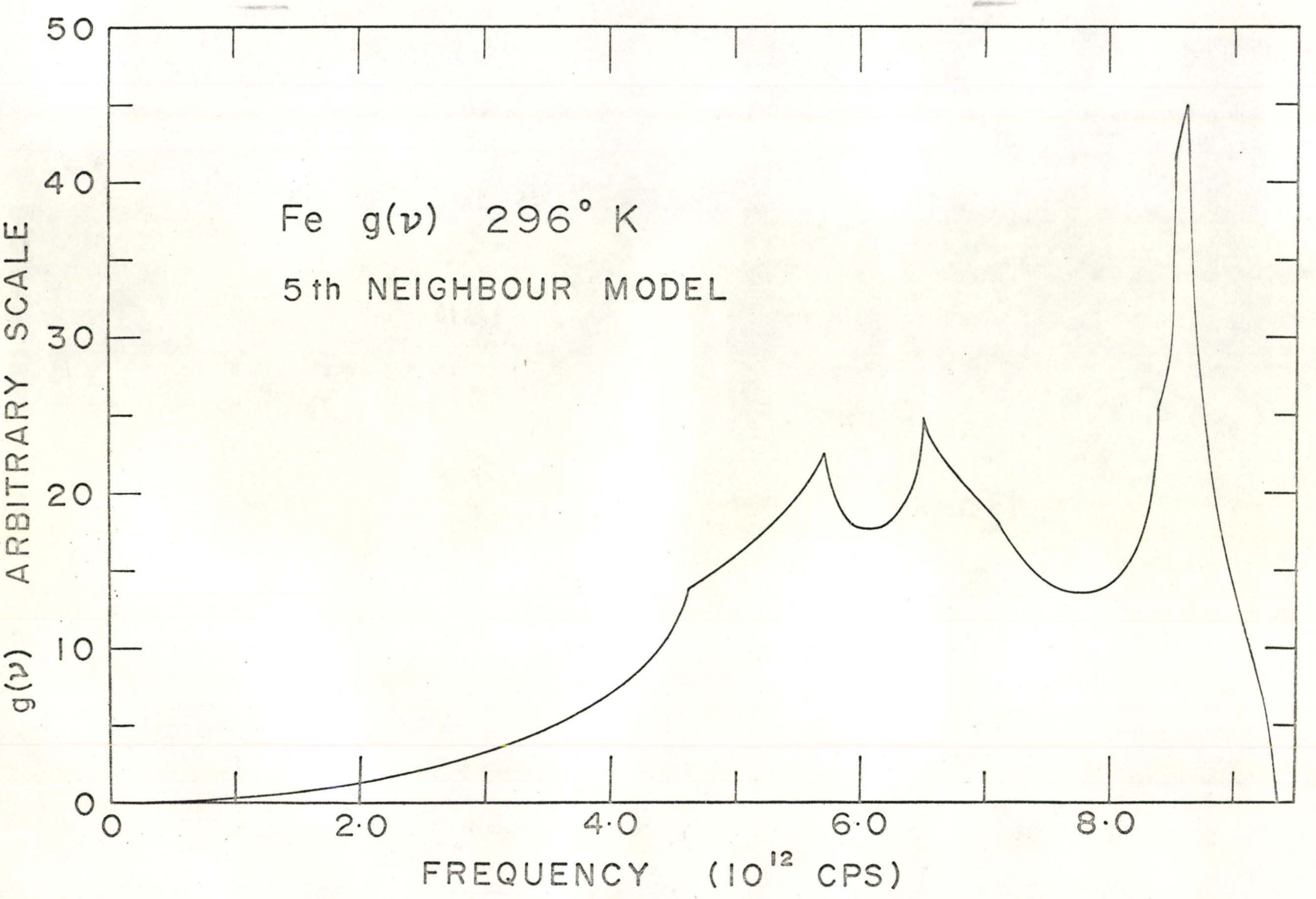

Fe g(ν) 296° K
5th NEIGHBOUR MODEL
g(ν) ARBITRARY SCALE
FREQUENCY (10^{12} CPS)
0
10
20
30
40
50
0
2·0
4·0
6·0
8·0

Fig. 7

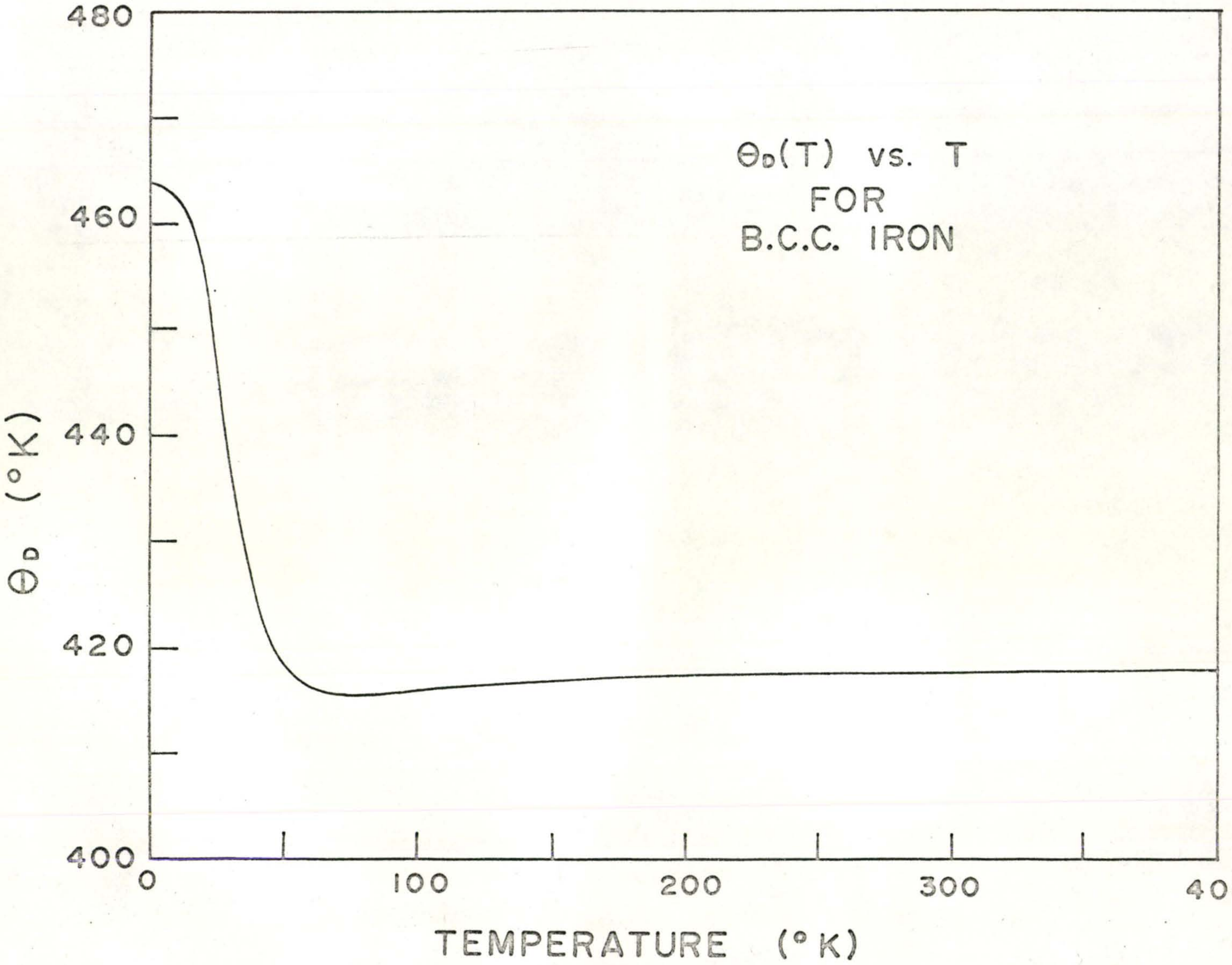

480
460
440
420
400
Θ_D (°K)
0
100
200
300
400
TEMPERATURE (°K)
$\Theta_D(T)$ vs. T
FOR
B.C.C. IRON

Fig. 9

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