

BR 8715737

ISSN 0101-3084

CNEN/SP

ipen Instituto de Pesquisas
Energéticas e Nucleares

DYNAMICAL PROPERTIES OF ALUMINIUM FROM EXPERIMENTAL
DISPERSION RELATIONS

João Batista Veiga Salles Filho, Roberto Fulfaro and Laercio Antonio Vinhas

IPEN - PUB -- 105

PUBLICAÇÃO IPEN 105

MAIO/1987

SÃO PAULO

**DYNAMICAL PROPERTIES OF ALUMINIUM FROM EXPERIMENTAL
DISPERSION RELATIONS**

José Batista Veiga Salles Filho, Roberto Fulfaro and Laercio Antonio Vinhas

DEPARTAMENTO DE FÍSICA E QUÍMICA NUCLEARES

**CNEN/SP
INSTITUTO DE PESQUISAS ENERGÉTICAS E NUCLEARES
SÃO PAULO - BRASIL**

Série PUBLICAÇÃO IPEN

INIS Categories and Descriptors

A13

ALUMINIUM
AXIAL SYMMETRY
DISPERSION RELATIONS
DYNAMICS
INELASTIC SCATTERING
NEUTRON SPECTROMETERS
THERMAL NEUTRONS

DYNAMICAL PROPERTIES OF ALUMINIUM FROM EXPERIMENTAL DISPERSION RELATIONS

João Batista Veiga Salles Filho, Roberto Fulfaro and Laercio Antonio Vinhas

ABSTRACT

Measurements of phonon dispersion relations of aluminium along the high symmetry directions were performed by coherent inelastic scattering of thermal neutrons technique. All measurements were taken at room temperature using the IPEN triple axis neutron spectrometer. The results obtained with accuracy are in good agreement with the published data.

The dispersion relations were calculated theoretically within the framework of Born-von Karman and Axially Symmetric models, including interactions up to the fifth nearest shell of atoms.

The elastic constants were determined using the values of sound propagating velocity obtained directly from the dispersion relations along of high symmetry directions of the crystal. Applying theoretical models the force constants of aluminium were also determined. From these data several physical properties of the metal can be obtained.

PROPRIEDADES DINÂMICAS DO ALUMÍNIO A PARTIR DE RELAÇÕES DE DISPERSÃO EXPERIMENTAIS

RESUMO

Foram medidas para a temperatura de 300 K, as relações de dispersão do alumínio nas direções de mais alta simetria do cristal, utilizando o espectrômetro de três eixos do IPEN. Os resultados mostraram-se precisos, com excelente concordância com alguns dados já existentes na literatura. Os cálculos teóricos das relações de dispersão foram efetuados com base nos modelos de dinâmica de redes de Born-von Karman e Axialmente Simétrico, tendo sido incluídas as interações até as cinco camadas de átomos mais próximas.

Os cálculos das constantes elásticas do alumínio foram efetuados a partir de valores da velocidade de propagação do som obtidos diretamente das curvas de dispersão, ao longo de certas direções de simetria do cristal. Por meio de aplicações dos modelos teóricos foram determinadas as constantes de força do alumínio, a partir das quais podem ser obtidas várias propriedades físicas desse metal.

I. INTRODUCTION

The study of the dynamical behaviour of crystalline structures is one of the most important applications of the neutron inelastic scattering technique. As part of the slow neutron inelastic scattering program of the Nuclear Physics Division of IPEN-CNEN/SP, a triple axis neutron spectrometer was built.

Details of the design and construction were object of a previous paper⁽³⁾. Measurements of the known dispersion relations of copper were also performed^(3,4,5), in order to verify the operational conditions and the performance of the instrument. The principal aim to be reached with these previous works was to present the main characteristics and details of the instrument and the difficulties and solutions found during its construction, as well as to acquire knowledge about the experimental techniques.

At the present, concerning the development of the lattice dynamics study program, the main interest is to obtain knowledge in the field of experimental data analysis and the application of theoretical models in order to determine physical properties in solids.

Therefore, from the experimental results of dispersion relations measured by using a monocrystalline sample of aluminium, the present study was developed. Its aim is the understanding of the main theoretical lattice vibration models applied to metals. Since there are well known and accurate dispersion relation data in the literature^(1,5), aluminium was chosen as matter of the study in order to simplify the approach of the present work.

The dispersion relations were calculated theoretically within the framework of Born-von Karman and Axially Symmetric models.

II. THEORY

II.1 – The Born-von Karman Model

The Born-von Karman lattice dynamical model has been described extensively by Born and Huang⁽²⁾. The following approximations are considered in this theory:

- The *adiabatic approximation*. The electrons are always able to adapt themselves to the instantaneous nuclear positions. The physical basis of the approximation considers that the ions, having a much larger mass, are moving much slower than the electrons. Concerning the dynamical aspects this means that the motions between electrons and ions can be separated. The valence electrons are able to give answer to perturbations in the plasma range times ($\tau \sim 10^{16}$ Hz), so the electrons will "effectively" follow the lattice motion instantaneously for all the frequencies of vibration.
- The *harmonic approximation*. The potential energy may be written as a general Taylor series in terms of the displacements of the atoms from their equilibrium positions. The atomic displacements μ are considered to be so small that the series expansion may be broken off after the quadratic term.
- The *requirement of periodic boundary conditions*. This is equivalent to replacing the finite specimen by an infinite medium, neglecting surface effects.

Let us consider the harmonic approximation for a solid with one atom per primitive cell, like aluminium (fcc). The primitive lattice translation vectors are represented by \vec{a} , \vec{b} and \vec{c} ; and the equilibrium positions by $\vec{r} = n\vec{a} + m\vec{b} + p\vec{c}$, where n , m and p are integers. The displacement of the ℓ -th atom from its equilibrium position is indicated by $\vec{\mu}_\ell$, being the position of the ℓ -th atom given by: $\vec{R}_\ell = \vec{r} + \vec{\mu}_\ell$.

Defining ϕ as the many body potential that governs the ion motion and expanding it in Taylor series in terms of the displacements $\vec{\mu}_\ell$, one obtains:

$$\phi = \phi_0 + \sum_{\ell} \sum_{\alpha} \phi_{\alpha}(\vec{r}) \mu_{\ell}^{\alpha} + \frac{1}{2} \sum_{\ell, \ell'} \sum_{\alpha, \beta} \phi_{\alpha\beta}(\vec{r}, \vec{r}') \mu_{\ell}^{\alpha} \mu_{\ell'}^{\beta} + \dots \quad (1)$$

where α is representing x , y or z and μ_{ℓ}^{α} is the Cartesian component α of $\vec{\mu}_{\ell}$ for an atom with mass equal to M .

The equilibrium potential ϕ_0 , corresponding to a static atomic lattice, may be taken as zero,

$$\phi_\alpha(\vec{r}) = \left. \frac{\partial \phi}{\partial \mu_\alpha} \right|_0 \quad \text{and} \quad \phi_{\alpha\beta}(\vec{r}, \vec{r}') = \left. \frac{\partial^2 \phi}{\partial \mu_\alpha \partial \mu_\beta} \right|_0 \quad (2)$$

The zero subscripts indicate that the derivatives are evaluated for the equilibrium configuration of the nuclei. At the equilibrium positions, where restoration force is zero, the second term in the second member of the equation⁽¹⁾, vanishes

From the translational invariance of the lattice it follows that: $\phi_{\alpha\beta}(\vec{r}, \vec{r}') = \phi_{\beta\alpha}(\vec{r}, \vec{r}') = \phi_{\alpha\beta}(\vec{r}-\vec{r}')$ and $\sum_{\vec{r}'} \phi_{\alpha\beta}(\vec{r}, \vec{r}') = 0$. The last expression is representing the fact that the resulting force in any atom is zero, if each atom is displaced from equilibrium by a displacement vector of same value.

In the harmonic approximation all terms beyond the harmonic term, i.e., the third term of the second member in equation⁽¹⁾ are neglected. Thus, the equation of motion for the atoms in the crystalline lattice can be written as:

$$M \ddot{\mu}_\alpha^\alpha = - \sum_{\vec{r}'} \sum_{\beta} \phi_{\alpha\beta}(\vec{r} - \vec{r}') \mu_\beta^\beta \quad (3)$$

Taking in account the periodic boundary conditions, one can define the normal coordinates Q_q , related with μ_α^α by:

$$\mu_\alpha^\alpha = \frac{1}{(NM)^{1/2}} \sum_q \mathbf{e}_q^\alpha Q_q e^{i\vec{q} \cdot \vec{r}} \quad (4)$$

where \vec{q} are the N primitive vectors⁽¹⁶⁾ that are placed within the first Brillouin zone, and \mathbf{e}_q^α are the polarization vectors. By substituting in eq.⁽³⁾, one obtains:

$$- \ddot{Q}_q \mathbf{e}_q^\alpha = Q_q \sum_{\beta} D_{\alpha\beta}(\vec{q}) \mathbf{e}_q^\beta \quad (5)$$

where $D_{\alpha\beta}(\vec{q})$ is an element of the dynamical matrix $D(\vec{q})$ given by:

$$D_{\alpha\beta}(\vec{q}) = \frac{1}{M} \sum_{\vec{r}} \phi_{\alpha\beta}(\vec{r}) e^{-i\vec{q} \cdot \vec{r}} \quad (6)$$

The frequencies of the waves described by Q_q are obtained from the eigenvalue equation per the polarization vectors \mathbf{e}_q^α :

$$\sum_{\beta} D_{\alpha\beta}(\vec{q}) \mathbf{e}_q^\beta = \omega^2 \mathbf{e}_q^\alpha \quad (7)$$

The three eigenvectors of $|D(\vec{q})|$ and the corresponding normal coordinates are indicated by $\mathbf{e}_{q\sigma}$ and by $Q_{q\sigma}$ ($\sigma = 1, 2, 3$).

In order to consider the polarization explicitly, equation⁽⁴⁾ must be modified and rewritten in the form

$$\vec{\mu}_\ell = \frac{1}{(NM)^{1/2}} \sum_{\vec{q}, \sigma} Q_{\vec{q}\sigma} \vec{e}_{\vec{q}\sigma} e^{i\vec{q} \cdot \vec{\ell}} \quad (8)$$

The Hamiltonian that corresponds to the equations of motion⁽³⁾ or the equivalent equation⁽⁵⁾ can be written in the diagonal form⁽⁶⁾

$$H = \frac{1}{2} \sum_{\vec{q}, \sigma} \left[\dot{Q}_{\vec{q}\sigma}^* \dot{Q}_{\vec{q}\sigma} + Q_{\vec{q}\sigma}^* Q_{\vec{q}\sigma} \omega^2(\vec{q}, \sigma) \right] \quad (9)$$

where

$$\omega^2(\vec{q}, \sigma) = (\vec{e}_{\vec{q}\sigma} | D(\vec{q}) | \vec{e}_{\vec{q}\sigma}) = \sum_{\alpha\beta} e_{\vec{q}\sigma}^\alpha D_{\alpha\beta}(\vec{q}) e_{\vec{q}\sigma}^\beta \quad (10)$$

From the definition of $D(\vec{q})$ in equation⁽⁵⁾, it is possible to verify that⁽⁷⁾

$$D(\vec{q} + \vec{G}) = D(\vec{q}) \quad (11)$$

where \vec{G} is a reciprocal lattice vector. Therefore $\omega^2(\vec{q})$ is periodic in the reciprocal lattice with a \vec{G} period.

By applying the translational invariance condition of the lattice, the interatomic force constants $\phi_{\alpha\beta}(\vec{\ell})$ can be written in the following form:

$$\phi_{\alpha\beta}(\vec{\ell}) = \left. \frac{\partial^2 \phi}{\partial \mu_\ell^\alpha \partial \mu_\ell^\beta} \right|_0 \quad (12)$$

since in the harmonic approximation the potential energy of a solid can be represented by a sum of the pair potentials $\phi(\vec{\ell}_1, \vec{\ell}_2)$, which depends only on the distance between the ions.

By substituting in eq.⁽⁵⁾, one can observe that

$$D_{\alpha\beta}(\vec{q}) = \frac{1}{M} \sum_{\vec{\ell}}' (1 - e^{-i\vec{q} \cdot \vec{\ell}}) \left. \frac{\partial^2 \phi}{\partial \mu_\ell^\alpha \partial \mu_\ell^\beta} \right|_0 \quad (13)$$

where the prime in the summation indicates that the term $\vec{\ell} = 0$ is excluded. The eq.⁽¹³⁾ is the basic result for the dynamical matrix in terms of the law of forces.

In the Born-von Karman model, the harmonic interaction between two atoms described in terms of a matrix of constants of tensorial forces, takes the following form⁽¹³⁾.

$$\phi_{\alpha\beta}^s = \begin{bmatrix} \alpha_1^s & & \beta_2^s \\ \beta_3^s & \alpha_2^s & \beta_1^s \\ \beta_2^s & \beta_1^s & \alpha_3^s \end{bmatrix} \quad (14)$$

where $\phi_{\alpha\beta}^s$ is the force applied along the "α" direction in an atom on the origin ($\vec{\ell} = 0$), when the sth neighbor atom is moving a unitary distance along the "β" direction.

This last expression, eq.⁽¹⁴⁾, giving the general form of the tensorial forces, will be used in the $\omega(\vec{q})$ function calculation.

11.2 – Axially Symmetric Model

In the Axially Symmetric Model⁽¹⁰⁾, the interaction potential between two atoms which have been displaced from equilibrium in a crystal is assumed to consist of two quadratic terms. The first is proportional to the square of the component of relative displacement along $\vec{\ell}$, the vector joining the equilibrium positions of the two atoms, and gives rise to a central or "bond-stretching" force. The second term is proportional to the square of the component of relative displacement perpendicular to $\vec{\ell}$ and causes a "bond-bending" force. Since all directions in the plane perpendicular to $\vec{\ell}$ are assumed to be equivalent, the interaction potential and corresponding forces are axially symmetric.

If $V(\vec{\ell})$ denotes the potential energy of interaction between two ions separated by a distance $|\vec{\ell}|$, then

$$V(|\vec{\ell} + \vec{\delta}|) = V(\ell) + V'(\ell) \frac{(\vec{\delta} \cdot \vec{\ell})}{\ell} + \frac{1}{2} V''(\ell) \frac{(\vec{\delta} \times \vec{\ell})^2}{\ell^3} + \frac{1}{2} V''(\ell) \frac{(\vec{\delta} \cdot \vec{\ell})^2}{\ell^3} + \text{higher terms in } \vec{\delta} \quad (15)$$

where ℓ is the magnitude of $\vec{\ell}$, $\vec{\delta}$ is an arbitrarily small vector displacement, and the primes on $V(\ell)$ denote differentiation with respect to ℓ . The term linear in $\vec{\delta}$ in eq.⁽¹⁵⁾ must be taken into account when considering the static stability of a lattice but can be neglected in determining the lattice vibrational spectrum. The third and fourth terms in the above equation are the pair bond-bending and bond-stretching contributions, respectively.

The force constants matrix can be referred to a system in which the main axis, for instance the X axis, is coincident with the line joining the two atoms. For this system, the matrix can be written in the following way:

$$\phi_{\alpha\beta}^s = \begin{pmatrix} A^s & 0 & 0 \\ 0 & B^s & 0 \\ 0 & 0 & B^s \end{pmatrix} \quad (16)$$

where $\phi_{\alpha\beta}^s$ has been defined previously.

This matrix, eq.⁽¹⁶⁾, will be used in the dynamical matrix calculation, eq.⁽¹³⁾, in order to determine the frequencies of the lattice vibrational modes by the axially symmetric model application.

The discussion about the Born-von Karman and Axially Symmetric models, shows the similarity between both calculations and also evidences a very simplified force constants matrix in the axially symmetric model, if compared with the matrix of the Born-von Karman model. This means that in the general case of an interaction of a given atom with the n-th nearest neighbor atoms, in the Born-von Karman model six force constants are necessary in order to represent the interaction, while in the Axially Symmetric model only two are necessary. So, since the solid allows the axial symmetry approximation for the interaction potential, it is clear that the Axially Symmetric model presents some advantage in order to represent the general case of interaction.

Nevertheless, in the Born-von Karman model it is possible to perform a reduction in the number of independent constants, for the case of a shell of atoms with them on the direction of the crystal lattice symmetry.

11.3 – Crystal Symmetry

By assuming $\vec{\ell}$ and \vec{L} as two vectors of the crystal lattice and both related by a unitary transformation "T", such as, $\vec{L} = T\vec{\ell}$, one can verify that if a given atom of \vec{L} is moving to $(\vec{L} + T\vec{\mu}q)$, thus the energy variation is the same as if the ion would move from $\vec{\ell}$ to $(\vec{\ell} + \vec{\mu}q)$. This can be represented by⁽¹⁴⁾:

$$[\phi_{\alpha\beta}(T\vec{\ell})] = (T_{ij}) [\phi_{\alpha\beta}(\vec{\ell})] (T_{ij})^* \quad (17)$$

where (T_{ij}) is a matrix that represents the unitary transformation "T" of the crystal lattice group of rotations.

Taking again the equation⁽⁶⁾ and b, considering the operation of transformation T over the wave vector of the crystal vibrations (\vec{q}), one obtains:

$$\begin{aligned} D_{\alpha\beta}(T\vec{q}) &= \frac{1}{M} \sum_{\vec{\ell}} \phi_{\alpha\beta}(\vec{\ell}) e^{-i T\vec{q} \cdot \vec{\ell}} \\ &= \frac{1}{M} \sum_{\vec{\ell}} \phi_{\alpha\beta}(\vec{\ell}) e^{-i \vec{q} \cdot T^* \cdot \vec{\ell}} \\ &= \frac{1}{M} \sum_{\vec{\ell}} \phi_{\alpha\beta}(T\vec{\ell}) e^{-i \vec{q} \cdot \vec{\ell}} \end{aligned} \quad (18)$$

the last above transformation follows from the fact that $T\vec{\ell}$ is a lattice crystal vector.

From equations 17 and 18 one verifies that:

$$[D(T\vec{q})] = (T_{ij}) [D(\vec{q})] (T_{ij})^*$$

Thus, $D(T\vec{q})$ and $D(\vec{q})$ are related by a unitary transformation, having the same eigenvalues. This means that $\omega^2(\vec{q})$ has the Brillouin zone symmetry; and it also shows that one can be aware of degenerescence of the lattice vibration frequency in symmetry positions to which there are operators "T" such as $T\vec{q} = \vec{q} + \vec{G}$, where \vec{G} is a reciprocal lattice vector.

In the present work, only the dispersion curves along the two directions of higher crystal symmetry will be considered in order to obtain the Aluminium force constants:

1. **Direction $\Delta \equiv (0,0,q)$:** the three polarization vectors for this direction are: (0,0,1), (0,1,0) and (1,0,0). The first vector indicates a pure longitudinal mode, while the two others indicate a degenerated transversal mode.
2. **Direction $\Sigma \equiv (q,q,0)$:** the three polarization vectors for this direction are: (1,1,0) (1, -1,0) and (0,0,1). The first vector indicates a pure longitudinal mode, while the two others indicate transversal modes, generally nondegenerated.

11.4 – Vibrational Dynamical Matrix for a Continuum Medium with Cubic Symmetry

The relations among crystal force constants and elastic constants can be obtained from a comparison between the solid crystal dynamical matrix and the vibrational dynamical matrix for a continuum medium, both assumed to be in the same symmetry

In a continuum medium, the force tensor (P_{ij}) and the deformation tensor (E_{ij}) are symmetrical having nine elements, from which six are independent. From the general form of the Hooke's law, each one of the (P_{ij}) nine elements are linearly related to the nine elements of (E_{ij}). Explicitly, the law, assumes that

$$P_{ij} = \sum_{\ell} \sum_{m} T_{ij\ell m} E_{\ell m} \quad (19)$$

where the constants $T_{ij\ell m}$ are forming a fourth order tensor.

Usually the deformations are denoted by the symbols e_{ij} , related to E_{ij} by the following expressions

$$\begin{aligned} e_{ii} &= E_{ii} \\ e_{ij} &= 2E_{ij}, \quad (i \neq j) \end{aligned} \quad (20)$$

being $E_{ij} = E_{ji}$. Indicating the displacement components (representing a deformation) by μ_1, μ_2 and μ_3 then the E_{ij} are defined by the equations⁽¹⁷⁾

$$\begin{aligned} e_{11} &= \frac{\partial \mu_1}{\partial x_1}, \quad e_{22} = \frac{\partial \mu_2}{\partial x_2}, \quad e_{33} = \frac{\partial \mu_3}{\partial x_3}, \quad e_{12} = \frac{\partial \mu_1}{\partial x_2} + \frac{\partial \mu_2}{\partial x_1}, \\ e_{21} &= \frac{\partial \mu_2}{\partial x_1} + \frac{\partial \mu_1}{\partial x_2}, \quad e_{13} = \frac{\partial \mu_1}{\partial x_3} + \frac{\partial \mu_3}{\partial x_1} \end{aligned} \quad (21)$$

where x_1, x_2 and x_3 are the cartesian components x, y and z , respectively.

In a medium presenting cubic symmetry, when the P_{ij} and $e_{\ell m}$ tensors are linearly related in agreement with the tensorial relation⁽¹⁹⁾, the C_{rs} coefficients of the deformation components in the six linear equations, give the following matrix:

$$\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix} \quad (22)$$

The C_{rs} coefficients are related to the elements of the $T_{ij,km}$ tensor, by:

$$\begin{aligned} C_{11} &= T_{11,11} \\ C_{12} &= T_{11,12} \\ C_{44} &= \frac{1}{2}(T_{23,23} + T_{23,32}) \end{aligned} \quad (23)$$

The amount of twenty one possible C_{rs} coefficients can be reduced to three independent coefficients as a consequence of keeping up invariant the tensorial form, eq.⁽¹⁹⁾, concerning the cube symmetry operations⁽⁸⁾. The coefficients C_{11} , C_{12} and C_{44} are the elastic constants for cubic crystals in the Voigt's notation⁽⁹⁾.

By substituting the eqs.⁽²¹⁾ in the linear relations between P_{ij} and e_{km} and by using the matrix of the eq.⁽²²⁾, one obtains

$$\begin{aligned} P_{ii} &= (C_{11} - C_{12}) \frac{\partial \mu_i}{\partial x_i} + C_{12} \left[\sum_{k=1}^3 \frac{\partial \mu_k}{\partial x_k} \right], \quad i = 1, 2, 3 \\ P_{ij} &= C_{44} \left[\frac{\partial \mu_i}{\partial x_j} + \frac{\partial \mu_j}{\partial x_i} \right], \quad i = 1, 2, 3, j = 2, 3 \text{ and } j > i \end{aligned} \quad (24)$$

The equilibrium conditions⁽⁷⁾ between the forces acting over a unitary volume, with mass equal to ρ and the P_{ij} surface forces, can be expressed as:

$$-\rho \frac{\partial^2 \mu_i}{\partial t^2} + \left[\sum_{k=1}^3 \frac{\partial P_{ik}}{\partial x_k} \right] = 0, \quad i = 1, 2, 3 \quad (25)$$

From the substitution of the eqs.⁽²⁴⁾ in eq.⁽²⁵⁾, the wave equations for crystals with cubic symmetry, can be obtained

$$\begin{aligned} \rho \frac{\partial^2 \mu_i}{\partial t^2} &= (C_{11} - C_{12}) \frac{\partial^2 \mu_i}{\partial x_i^2} + C_{12} \left[\sum_{k=1}^3 \frac{\partial^2 \mu_k}{\partial x_i \partial x_k} \right] + \\ &+ C_{44} \left[\sum_{j=1}^3 \left(\frac{\partial^2 \mu_i}{\partial x_j^2} + \frac{\partial^2 \mu_j}{\partial x_i \partial x_j} \right) \right], \quad i = 1, 2, 3 \end{aligned} \quad (26)$$

In order to solve the above equations, the equation for a plane wave must be considered:

$$\mu_j = A_j \exp [i(\omega t - \vec{q} \cdot \vec{x})], \quad j = 1, 2, 3, \dots \quad (27)$$

From this substitution, a system of three homogenous equations in A_1 , A_2 , A_3 , is obtained:

$$\begin{aligned} &[(C_{11} - C_{44})q_1^2 + C_{44}q^2 - \rho\omega^2] A_1 + (C_{12} + C_{44})q_1 q_2 A_2 + \\ &+ (C_{12} + C_{44})q_1 q_3 A_3 = 0 \\ &(C_{12} + C_{44})q_1 q_2 A_1 + [(C_{11} - C_{44})q_2^2 + C_{44}q^2 - \rho\omega^2] A_2 + \\ &+ (C_{12} + C_{44})q_2 q_3 A_3 = 0 \\ &(C_{12} + C_{44})q_1 q_3 A_1 + (C_{12} + C_{44})q_2 q_3 A_2 + [(C_{11} - C_{44})q_3^2 + \\ &+ C_{44}q^2 - \rho\omega^2] A_3 = 0 \end{aligned} \quad (28)$$

where $q^2 = q_1^2 + q_2^2 + q_3^2$.

The condition for solving the set of equations above, is:

$$\det [D(\vec{q}) - \rho\omega^2 I] = 0 \quad (29)$$

where I is the identity matrix and $D(\vec{q})$ is a dynamical matrix for a continuum medium with cubic symmetry (for a large wavelength limit) represented by

$$D(\vec{q}) = \begin{pmatrix} (C_{11} - C_{44})q_1^2 + C_{44}q^2 & (C_{12} + C_{44})q_1q_2 & (C_{12} + C_{44})q_1q_3 \\ (C_{12} + C_{44})q_1q_2 & (C_{11} - C_{44})q_2^2 + C_{44}q^2 & (C_{12} + C_{44})q_2q_3 \\ (C_{12} + C_{44})q_1q_3 & (C_{12} + C_{44})q_2q_3 & (C_{11} - C_{44})q_3^2 + C_{44}q^2 \end{pmatrix} \quad (30)$$

In the sequence of the present work the $D(\vec{q})$ matrix will be used in order to obtain the relations between the elastic constants and the force constants for aluminium. From the knowledge of this relations it is possible to determine the force constants by the Born-von Karman model.

III. EXPERIMENTAL RESULTS AND DATA ANALYSIS

By using the IPEN-CNEN/SP triple axis neutrons spectrometer⁽³⁾, the dispersion relation, $\omega = \omega(\vec{q})$, of aluminium was measured, at room temperature, along the two directions of higher symmetry of the fcc crystal lattice: $\Delta \equiv (00\xi)$ direction and $\Sigma \equiv (\xi\xi 0)$ direction. In the present work the mode of operation of the spectrometer was the "constant Q" method^(4,5,12) in which the momentum transfer is kept constant while an energy distribution is obtained.

In the experiments, coherent one-phonon scattering processes occur preferentially, in which the energy and momentum of the neutrons are changed from their initial values, E_0 and $\hbar\vec{k}_0$ to final values E_1 and $\hbar\vec{k}_1$ governed by the conservation conditions:

$$E_0 = E_1 + \hbar\omega_1(\vec{q}) \quad (31)$$

$$\vec{k}_0 - \vec{k}_1 = \vec{q} + \vec{G} = \vec{Q} \quad (32)$$

where \vec{Q} is the momentum transfer vector, \vec{q} the reduced wave vector of the phonon involved in the scattering process, and \vec{G} a vector of the reciprocal lattice previously mentioned. Peaks are obtained when the frequency ω given by eq.⁽³¹⁾ coincides with that of the phonon whose wave vector is \vec{q} , given by eq.⁽³²⁾. This process is repeated for successive values of \vec{q} along high-symmetry directions in the crystal. Such measurements provide direct information concerning the interatomic forces.

The several experimental points of the aluminium dispersion relation⁽¹²⁾, measured along the (00ξ) and $(\xi\xi 0)$ higher symmetry directions, are represented in Figure 1 by full squares. These points, obtained by using the IPEN-CNEN/SP spectrometer, are coincident with the experimental data for aluminium measured by Yarnell et alii⁽¹⁵⁾. These authors kindly agreed to send us their results, through private communication, in order to be used together with our results in the calculations of the present work.

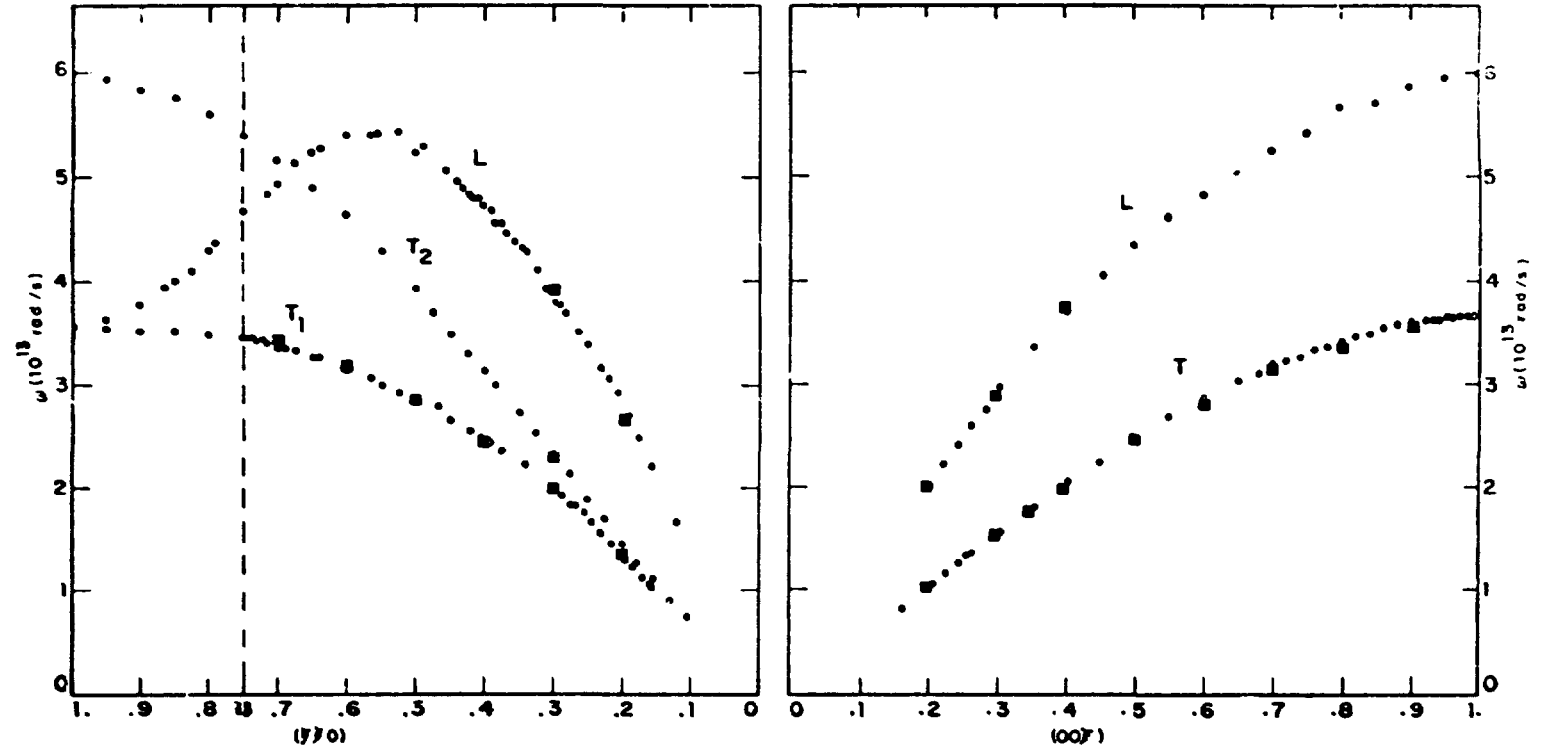


Figure 1 - Dispersion Curves for Aluminium, at Room Temperature

III.1 – Velocity of Sound and Elastic Constants Calculation

The velocity of propagation of sound and elastic constants are physical properties of a solid that can be obtained directly from the experimental dispersion relation. Simple expressions relating elastic constants to the velocity of sound and the material density ρ can be achieved by choosing in an appropriate way the directions of propagation and of polarization. For this purpose it is only necessary to substitute the selected \vec{q} and \vec{A} values in the equations⁽²⁸⁾

For long wavelength, where the dispersion is not present, the velocity of sound is given by⁽¹⁶⁾

$$v = \frac{\omega}{q} \quad (33)$$

The (00ξ) and $(\xi\xi 0)$ are two of possible propagation directions that give the mentioned simple relations. For a plane wave on the (00ξ) direction, one has $q_3 = q$ and $q_1 = q_2 = 0$. Thus, $A_3 = A$ and $A_1 = A_2 = 0$ describes a longitudinal wave. The velocity of sound is given by:

$$\rho V_L^2 = C_{11} \quad (34)$$

For transversal plane waves ($A_3 = 0$), polarized in any direction perpendicular to X_3 (or Z) axis, the velocity V_T is given by:

$$\rho V_T^2 = C_{44} \quad (35)$$

For the $(\xi\xi 0)$ direction one has that $q_1 = q_2 = q/\sqrt{2}$ and $q_3 = 0$. The V_L velocity of a longitudinal wave ($A_3 = 0$) is written as:

$$\rho V_L^2 = \frac{1}{2}(C_{11} + C_{12} - 2C_{44}) \quad (36)$$

The V_{T1} velocity of a transversal wave, polarized in a direction perpendicular to X_3 (or Z) axis, ($A_3 = 0$) is given by:

$$\rho V_{T1}^2 = \frac{1}{2}(C_{11} - C_{12}) \quad (37)$$

The velocity V_{T2} of a transversal wave, polarized in a direction parallel to the X_3 axis ($A_1 = A_2 = 0$) is given by:

$$\rho V_{T2}^2 = C_{44} \quad (38)$$

The velocity of propagation of sound for the (00ξ) and $(\xi\xi 0)$ directions in all the polarizations, was determined from Figure 1, in the long wavelength range (small \vec{q}), where the variation of ω with respect to \vec{q} is linear, in agreement with what is foreseen by equation⁽³⁵⁾.

Table I presents the values determined for the velocity of sound propagating along the mentioned directions.

Table I

Direction	Polarization	Velocity of Sound (cm/s)
(00 ζ)	L	$V_L = (6.3 \pm 0.2) \cdot 10^5$
	T	$V_T = (3.3 \pm 0.1) \cdot 10^5$
$(\zeta\zeta 0)$	L	$V_L = (6.5 \pm 0.2) \cdot 10^5$
	T ₁	$V_{T_1} = (3.0 \pm 0.1) \cdot 10^5$
	T ₂	$V_{T_2} = (3.2 \pm 0.1) \cdot 10^5$

From the values of Table I and by considering $\rho = 2.702 \text{ g/cm}^3$ for the aluminium density, the system of equations (36), (37) and (38) can be solved in order to determine the values for C_{11} , C_{12} and C_{44} .

Table II presents (in units of $10^{11} \text{ dynes/cm}^2$) the results of the present work for the elastic constants determination, as well as those existing in the literature⁽¹³⁾.

Table II

	Present Work	Literature
C_{11}	11.0 ± 0.6	10.92
C_{12}	6.2 ± 0.3	6.40
C_{44}	2.8 ± 0.1	3.04

III.2 – Force Constants Calculation

In order to obtain the aluminium force constants, from the experimental dispersion relations Born-von Karman and Axially Symmetric theoretical models were used.

III.2.1 – Born-von Karman model

Dispersion relation analysis is made by assuming the harmonic approximation.

In the determination of the crystal force constants values it is necessary to fit a $\omega = \omega(\vec{q})$ function to the experimental dispersion relation. This function is provided by the theoretical model, having the force constants included as parameters

The theoretical function to be searched for is a solution of the eigenvalues equation⁽⁷⁾. In order to find the matrix element $\phi_{\alpha\beta}(\vec{\ell})$ included in equation⁽¹³⁾ it is necessary to use equation⁽¹⁷⁾, which can be calculated in a any lattice point, with the condition that $[\phi_{\alpha\beta}(\vec{\ell})]$ is known in a given particular lattice point and the matrix representing the rotation operation between these points $[T_{ij}]$ is also known. The force constants matrix $[\phi_{\alpha\beta}(\vec{\ell})]$ is of order three and it has nine elements, being six of them independent.

The crystal symmetry allows reducing the number of these elements. To do this, a unitary transformation $[T_{ij}]$ that does not change the atoms positions in $\vec{\ell}$ and $\vec{\ell}'$, is considered; thus, the matricial relation that allows reducing the elements of the force constants matrix, can be written in the form.

$$[\phi_{\alpha\beta}(\vec{\ell} - \vec{\ell}')] = (T_{ij}) [\phi_{\alpha\beta}(\vec{\ell} - \vec{\ell}')] (T_{ij})^t \quad (39)$$

Let us consider a face centered cubic lattice (like the aluminium case) and assume only the interactions between the nearest atoms or the first shell of atoms. It is useful to perform this last assumption, since the calculations where the interactions between the atom and the s^{th} shell of atoms are considered, is made in a similar way⁽¹²⁾.

By assuming the interaction between "0" atom and "1" atom, one can represent this case in the tensorial general form, as below:

$$\phi^1(0,1) = \begin{pmatrix} \alpha_1^1 & \beta_3^1 & \beta_2^1 \\ \beta_3^1 & \alpha_2^1 & \beta_1^1 \\ \beta_2^1 & \beta_1^1 & \alpha_3^1 \end{pmatrix} \quad (40)$$

The first neighbor coordinate is (a,a,0). By performing the two crystal symmetry operations (reflections in xy and x = y planes) that keeping up invariant the vector (a,a,0) joining the two atoms, one can obtain the force constants matrix that represents the interaction between "0" and "1" atoms. The matrix can be written in the simplified irreducible form:

$$\phi^1(0,1) = \begin{pmatrix} \alpha_1^1 & \beta_3^1 & 0 \\ \beta_3^1 & \alpha_1^1 & 0 \\ 0 & 0 & \alpha_3^1 \end{pmatrix} \quad (41)$$

From equation⁽¹⁷⁾ it is possible to find the force constants matrix for the interaction between the "0" atom and each one of the eleven remaining atoms on the shell⁽¹²⁾.

From the obtained results, one is able to calculate the dynamical matrix element $D_{11}^1(\vec{q})$, by using equation⁽¹³⁾.

$$D_{11}^1(\vec{q}) = \frac{4}{M} [\alpha_1^1 (2 - \cos q_x \cdot \cos q_y - \cos q_x \cdot \cos q_z) + \alpha_3^1 (1 - \cos q_y \cdot \cos q_z)]$$

The other dynamical matrix elements are obtained by performing similar calculations.

$$D_{12}^1(\vec{q}) = \frac{4}{M} \{ \alpha_1^1 (2 - \cos q_x \cos q_y \cos q_z) + \alpha_3^1 (1 - \cos q_x \cos q_z) \}$$

$$D_{13}^1(\vec{q}) = \frac{4}{M} \{ \alpha_1^1 (2 \cos q_x \cos q_z \cos q_y \cos q_z) + \alpha_3^1 (1 - \cos q_x \cos q_z) \}$$

$$D_{12}^1(\vec{q}) = D_{21}^1(\vec{q}) = \frac{4}{M} \beta_1^1 \sin q_x \sin q_y$$

$$D_{13}^1(\vec{q}) = D_{31}^1(\vec{q}) = \frac{4}{M} \beta_3^1 \sin q_x \sin q_z$$

$$D_{23}^1(\vec{q}) = D_{32}^1(\vec{q}) = \frac{4}{M} \beta_3^1 \sin q_y \sin q_z$$

Table III shows the force constants matrices for the first five shell of atoms, with explicit indication as to the interaction to which the matrix is referred.

Table III

Shell	Coordinate of Atom that is Interacting with Atom in (0,0,0)	Force Constant Matrix	Nº of Atoms in the Shell
1	(a, a, 0)	$\begin{bmatrix} \alpha_1^1 & \beta_3^1 & 0 \\ \beta_3^1 & \alpha_1^1 & 0 \\ 0 & 0 & \alpha_3^1 \end{bmatrix}$	12
2	(2a, 0, 0)	$\begin{bmatrix} \alpha_1^2 & 0 & 0 \\ 0 & \alpha_2^2 & 0 \\ 0 & 0 & \alpha_3^2 \end{bmatrix}$	6
3	(2a, a, a)	$\begin{bmatrix} \alpha_1^3 & \beta_2^3 & \beta_3^3 \\ \beta_1^3 & \alpha_2^3 & \beta_2^3 \\ \beta_2^3 & \beta_1^3 & \alpha_2^3 \end{bmatrix}$	24
4	(2a, 2a, 0)	$\begin{bmatrix} \alpha_1^4 & \beta_3^4 & 0 \\ \beta_3^4 & \alpha_1^4 & 0 \\ 0 & 0 & \alpha_3^4 \end{bmatrix}$	12
5	(3a, a, 0)	$\begin{bmatrix} \alpha_1^5 & \beta_3^5 & 0 \\ \beta_3^5 & \alpha_1^5 & 0 \\ 0 & 0 & \alpha_3^5 \end{bmatrix}$	24

The element $D_{ij}^s(\vec{q})$ of the Born-von Karman dynamical matrix, that corresponds to interactions up to the fifth shell of atoms, is given by:

$$D_{ij}^s(\vec{q}) = \sum_{s=1}^5 D_{ij}^s(\vec{q}) \quad (42)$$

where $D_{ij}^s(\hat{q})$ is the (i,j) element of the dynamical matrix for interactions between the atom in the origin and the S^{th} shell of atoms. Therefore, from equation(42) one can write:

$$\begin{aligned}
 D_{11}(\hat{q}) = & \frac{1}{M} [4\alpha_1^4 (2 - \cos q_x \cos q_y - \cos q_x \cos q_z) + 4\alpha_3^4 (1 - \cos q_y \cos q_z) + \\
 & + 2\alpha_2^4 (2 - \cos 2q_y - \cos 2q_z) + 8\alpha_1^3 (1 - \cos 2q_x \cos q_y \cos q_z) + \\
 & + 8\alpha_2^3 (2 - \cos q_x \cos 2q_y \cos q_z - \cos q_x \cos q_y \cos 2q_z) + \\
 & + 4\alpha_1^4 (2 - \cos q_x \cos q_y - \cos q_x \cos q_z) + 4\alpha_3^4 (1 - \cos q_y \cos q_z) + \\
 & + 4\alpha_1^5 (2 - \cos 3q_x \cos q_y - \cos 3q_x \cos q_z) + 4\alpha_2^5 (2 - \cos q_x \cos 3q_y - \cos q_x \cos 3q_z) + \\
 & + 4\alpha_3^5 (2 - \cos q_y \cos 3q_z - \cos 3q_y \cos q_z)]
 \end{aligned} \tag{43}$$

$$\begin{aligned}
 D_{12}(\hat{q}) = & \frac{1}{M} [4\beta_3^3 \sin q_x \sin q_y + 8\beta_1^3 \sin q_x \sin q_y \cos 2q_y + \\
 & + 8\beta_2^3 (\sin 2q_x \sin q_y \cos q_z + \sin q_x \sin 2q_y \cos q_z) + 4\beta_3^4 \sin q_x \sin q_y + \\
 & + 4\beta_2^5 (\sin 3q_x \sin q_y + \sin q_x \sin 3q_y)]
 \end{aligned} \tag{44}$$

The element D_{22} (D_{33}) can be found from D_{11} (D_{22}) by changing x by q , y by z and z by x . In a similar way, the element D_{23} (D_{13}) also can be obtained from D_{12} (D_{23}) by a cyclical permutation of x , y and z . It is convenient to point out that the matrix is symmetric.

III.2.2 – Axially Symmetric Model

In this model there are two axially symmetric constants for each shell of atoms assumed in the interaction.

For sake of simplicity, the axially symmetric force constants are obtained in function of the tensorial force constants, since this procedure allows the utilization of the dynamical matrix calculated for the Born-von Karman model (or tensorial).

For interactions up to the first shell of atoms, the relation between these force constants can be obtained by assuming the interaction between the "0" atom and the "1" atom, by performing a 45° rotation around the z axis, in such a way that the x axis stays coincident with the direction joining these atoms.

The matrix that performs the rotation is given by:

$$T_{(45)} = \begin{pmatrix} \sqrt{\frac{2}{2}} & \sqrt{\frac{2}{2}} & 0 \\ -\sqrt{\frac{2}{2}} & \sqrt{\frac{2}{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (45)$$

When a rotation is applied to the $\phi^1(0,1)$ matrix given by the equation(41), one obtains:

$$\begin{pmatrix} \sqrt{2/2} & \sqrt{2/2} & 0 \\ -\sqrt{2/2} & \sqrt{2/2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1^1 & \beta_3^1 & 0 \\ \beta_3^1 & \alpha_1^1 & 0 \\ 0 & 0 & \alpha_3^1 \end{pmatrix} \begin{pmatrix} \sqrt{2/2} & \sqrt{2/2} & 0 \\ \sqrt{2/2} & \sqrt{2/2} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \alpha_1^1 + \beta_3^1 & 0 & 0 \\ 0 & \alpha_1^1 - \beta_3^1 & 0 \\ 0 & 0 & \alpha_3^1 \end{pmatrix} \quad (46)$$

By comparing the (45) and (46) matrices and in order to have axially symmetric forces, one must have:

$$\alpha_3^1 = \alpha_1^1 - \beta_3^1 \quad (47)$$

where axially symmetric force constants are given in function of tensorial force constants, such as:

$$A^1 = \alpha_1^1 + \beta_3^1 \text{ and } B^1 = \alpha_1^1 - \beta_3^1$$

Expression (47) is the restriction of the axially symmetric model to the tensorial force constants, for interactions up to the first shell of atoms

Table IV shows (for the five first shell of atoms centered at origin) the tensorial force constants, the restrictions imposed to them by the Axially Symmetric model and the axially symmetric force constants.

According to what was previously mentioned, in order to obtain the theoretical function $\omega = \omega(\vec{q})$ it is necessary to solve the eigenvalue equation (7). This task becomes easier when the function is calculated for the crystal directions of higher symmetry. For aluminium (fcc) these directions are: (00ζ) and $(\zeta\zeta 0)$.

In order to obtain the eigenvalue of the $|D(\vec{q})|$ matrix for each one of the mentioned directions, it is enough a multiplication by the correspondent eigenvector of each excited mode.

Table V shows the eigenvectors for the five branches of the experimental dispersion relation.

Let us write the dynamical matrix in the following form:

$$D(\vec{q}) = \begin{pmatrix} D_{11} & D_{12} & D_{13} \\ D_{12} & D_{22} & D_{23} \\ D_{13} & D_{23} & D_{33} \end{pmatrix}$$

where, by simplicity, the indication of the dependence of each element with \vec{q} was suppressed.

Table IV

FORCE CONSTANTS			
Shell	Tensorial Model (Born-von Karman)	Axially Symmetric Model Restrictions	Axially Symmetric Model
1	α_1^1 α_3^1 β_3^1	$\alpha_3^1 = \alpha_1^1 - \beta_3^1$	A^1 B^1
2	α_1^2 α_2^2	-	A^2 B^2
3	α_1^3 α_2^3 β_1^3 β_2^3	$\beta_1^3 = \frac{1}{3}(\alpha_1^3 - \alpha_2^3)$ $\beta_2^3 = \frac{2}{3}(\alpha_1^3 - \alpha_2^3)$	A^3 B^3
4	α_1^4 α_3^4 β_3^4	$\alpha_3^4 = \alpha_1^4 - \beta_3^4$	A^4 B^4
5	α_1^5 α_2^5 α_3^5 β_3^5	$\alpha_3^5 = \frac{1}{8}(9\alpha_2^5 - \alpha_1^5)$ $\beta_3^5 = \frac{3}{8}(\alpha_1^5 - \alpha_2^5)$	A^5 B^5

Table V

Direction	Polarization	Eigenvector
(00 ζ)	L	(0,0,1)
	T	(0,1,0) (1,0,0)
$(\zeta\zeta 0)$	L	(1,1,0)
	T ₁	(1,-1,0)
	T ₂	(0,0,1)

For a phonon that is propagating along the (00 ζ) ($q_x = q_y = 0$) direction, the dynamical matrix can be written in the diagonal form

$$D(\vec{q}) = \begin{vmatrix} D_{11} & 0 & 0 \\ 0 & D_{11} & 0 \\ 0 & 0 & D_{33} \end{vmatrix}$$

where the square of the frequency of the longitudinal mode (ω_L^2) is given by:

$$\omega_L^2 \begin{vmatrix} 0 & 0 & 0 \\ 0 & D_{11} & 0 \\ 1 & 0 & D_{33} \end{vmatrix} = \begin{vmatrix} D_{11} & 0 & 0 \\ 0 & D_{11} & 0 \\ 0 & 0 & D_{33} \end{vmatrix} \begin{vmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 1 \end{vmatrix} \quad (48)$$

$$= \begin{vmatrix} D_{11} & 0 \\ 0 & D_{33} \end{vmatrix} \begin{vmatrix} 0 & 0 \\ 0 & 1 \end{vmatrix}$$

$$\omega_L^2 = D_{33}$$

and the transversal mode by:

$$\omega_T^2 = D_{11} \quad (49)$$

From the theory one can obtain two transversal modes, but in the case of (00 ζ) direction these modes are degenerated, as can be seen by solving the eigenvalue equation for the (0,1,0) eigenvector.

In analogy, for a phonon propagating along the ($\zeta\zeta$ 0) ($q_x = q_y$ and $q_z = 0$), the dynamical matrix can be written in the form

$$D(\vec{q}) = \begin{vmatrix} D_{11} & D_{12} & 0 \\ D_{12} & D_{11} & 0 \\ 0 & 0 & D_{33} \end{vmatrix}$$

the square of the frequencies of the longitudinal (ω_L^2) and transversal ($\omega_{T_1}^2$ and $\omega_{T_2}^2$) modes, are given by:

$$\omega_L^2 = D_{11} + D_{12} \quad (50)$$

$$\omega_{T_1}^2 = D_{11} - D_{12} \quad (51)$$

e

$$\omega_{T_2}^2 = D_{33} \quad (52)$$

In the (00 ζ) and ($\zeta\zeta$ 0) directions, the functions (48) to (52) are relating the $\omega = \omega(\vec{q})$ curve with the crystal force constants. From this, it is possible to obtain the crystal force constants by performing a fit of each mentioned function with the respective branch of the experimental curve, by the application of the non linear least-square method⁽¹¹⁾.

Since each parameter of the $\omega = \omega(\vec{q})$ function is a linear combination of force constants, a system of equations where crystal force constants are the unknown values, is produced when the least-squares method is applied. For interactions between the atom on the origin with the atoms on the five nearest shells, the Born-von Karman model gives an indetermined linear system, when the (00ζ) and $(\zeta\zeta 0)$ directions are considered. In order that the system has a unique solution, one must add to the system independent linear equations relating force constants with elastic constants.

By assuming the limit for long wavelength (small values for wavevector \vec{q}) in the crystal dynamical matrix and by comparing it with the dynamical matrix in a continuum medium with cubic symmetry (eq. (30)), one can obtain the following relations between force and elastic constants:

$$\begin{aligned}
 2aC_{11} &= 4\alpha_1^1 + 4\alpha_1^2 + 16\alpha_1^3 + 8\alpha_2^3 + 16\alpha_1^4 + 36\alpha_1^4 + 4\alpha_2^5 \\
 2aC_{44} &= 2\alpha_1^1 + 2\alpha_3^1 + 4\alpha_2^2 + 4\alpha_1^3 + 20\alpha_2^3 + 8\alpha_1^4 + 8\alpha_1^4 + 2\alpha_1^5 + 18\alpha_2^5 + 20\alpha_3^5 \\
 2a(C_{12} + C_{44}) &= 4\beta_1^1 + 8\beta_1^3 + 32\beta_2^3 + 16\beta_3^4 + 24\beta_3^5
 \end{aligned} \tag{53}$$

where $2a$ is the fcc cubic lattice parameter.

Table VI shows the values of the tensorial force constants as well as the values of the axially symmetric force constants, obtained for aluminium by the Born-von Karman and Axially Symmetric Modes, respectively.

This table presents the values for force constants of the tensorial and axially symmetric types, obtained from experimental dispersion curves of aluminium, measured at 300 K. For the application of the models were considered the interactions between the atom on the origin with the atoms on the five nearest shells. The third and fourth columns are showing the results for tensorial force constants obtained by using the Born-von Karman and Axially Symmetric models, respectively. A comparison between the values in both columns is showing that they are not coincident, however in the determination of the parameters of the lattice vibration frequency function, a linear combination of the mentioned values is used. This last cited function is utilized in order to reproduce theoretically the dispersion relations, whose calculated curves by the models application can be seen in Figure 2 in good agreement with the experimental points.

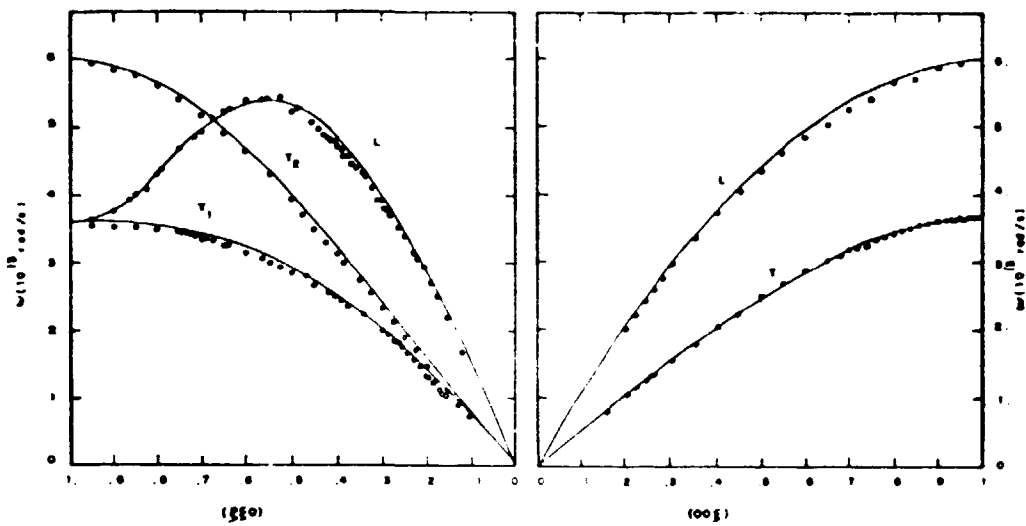
Figure 2 is showing the calculated dispersion relation for aluminium, obtained from the application of the Born-von Karman and Axially Symmetric models, by assuming interactions between the atom on the origin and the atoms on the five nearest shells.

The results of the calculation of Axially Symmetric model application are showing that for aluminium the axial symmetry can be used for the interatomic forces study. The fifth column of Table VI presents the obtained values for the axially symmetric force constants calculated from the Axially Symmetric model and the Figure 2 shows the dispersion relation for aluminium at 300 K calculated in the $(\zeta\zeta 0)$ and (00ζ) directions by the application of the mentioned models, as well as the experimental points obtained by Yarnell et al⁽¹⁵⁾.

Table VI

Shell	FORCE CONSTANTS (dines/cm)			
		Tensorial		Axially Symmetric
		Born-von Karman Model	Axially Symmetric Model	Axially Symmetric Model
1	α_1^1	10253	10004	---
	α_3^1	2549	-1903	---
	β_3^1	10570	11907	---
	A^1	---	---	21911
	B^1	---	---	-1903
2	α_1^2	2806	2828	---
	α_2^2	1740	1426	---
	A^2	---	---	2828
	B^2	---	---	1426
3	α_1^3	113	-169	--
	α_2^3	-300	-256	--
	β_1^3	156	29	--
	β_2^3	27	58	--
	A^3	--	--	-111
	B^3	--	--	-285
4	α_1^4	-591	-547	--
	α_3^4	-44	-19	--
	β_3^4	-340	-528	--
	A^4	--	--	-1075
	B^4	--	--	-19
5	α_1^5	282	282	--
	α_2^5	77	33	--
	α_3^5	-43	2	--
	β_3^5	0	93	--
	A^5	--	--	313
	B^5	--	--	2

Born-von Karman Model



Axially Symmetric Model

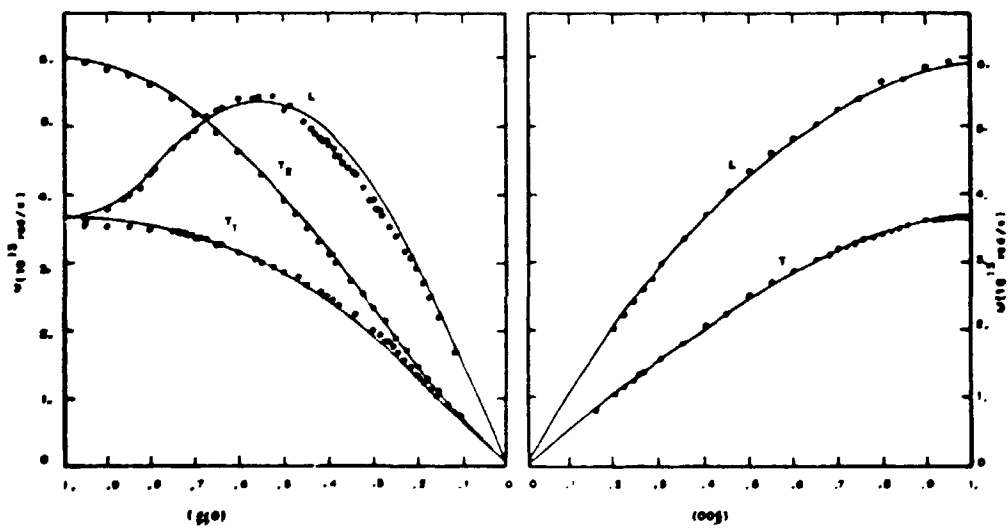


Figure 2 – Dispersion Relations Calculated by the Born-von Karman and Axially Symmetric Models

REFERENCES

1. ASHCROFT, N. W. & MERMIN, N. D. *Solid state physics*. New York, Wiley 1975.
2. BORN, M. & HUANG, K. *Dynamical theory of crystal lattices*. London Oxford, 1954.
3. FUHRMANN, C. *Projeto e construção de um espectrômetro de cristal de três eixos para nêutrons e verificação do desempenho por meio da medida das relações de dispersão do cobre*. São Paulo, 1979. (Dissertação de Mestrado, Instituto de Energia Atômica).
4. FUHRMANN, C.; FULFARO, R.; VINHAS, L. A. *Desempenho do espectrômetro de cristal de três eixos do IEA: medida das relações de dispersão do cobre*. São Paulo, Instituto de Energia Atômica, abr., 1978. (IEA-504; COURP-AFM-63)
5. FULFARO, R.; VINHAS, L. A.; PUGLIESI, R. *Focusing conditions in neutron inelastic scattering experiments with the IPEN tripleaxis spectrometer*. São Paulo, Instituto de Pesquisas Energéticas e Nucleares, Oct. 1980. (IPEN-20)
6. HARDY, J. R. Phenomenological models in lattice dynamics. In: MARADUDIN, A. A. & Horton, E. K. eds. *Dynamical properties of solids V.1: crystalline solids fundamentals*. Amsterdam, North Holland, 1974. p.1-82.
7. JOOS, G. *Theoretical physics*. London, Blackie, 1959.
8. KITTEL, C. *Introduction to solid state physics*. New York, Academic, 1965.
9. KOSTER, G. F. Space groups and their representations. *Solid State Phys.*, 5:173-256, 1957.
10. LEHMAN, G. N.; WOLFRAM, T.; DE WAMES, R. E. Axially symmetric model for lattice dynamics of metals with application to Cu Al and Zr. *H. Phys. Rev.*, 128:1593, 1962.
11. McCALLA, T. R. *Introduction to numerical methods and FORTRAN programming*. New York, Wiley, 1967.
12. SALLES FILHO, J. B. V. *Estudos da dinâmica de rede do alumínio por meio de espalhamento inelástico de nêutrons*. São Paulo, 1982. (Dissertação de Mestrado, Instituto de Pesquisas Energéticas e Nucleares)
13. SQUIRES, G. L. The relation between the interatomic forces and the frequencies of symmetric phonons in cubic crystals. In: INTERNATIONAL ATOMIC ENERGY AGENCY. *Inelastic scattering of neutrons in solids and liquids: proceedings of the symposium on . . . , held in Chalk River, Canada. 10-14, Spt., 1962*. Vienna 1963 p.71-86
14. TINKHAM, M. *Group theory and quantum mechanics*. New York, McGraw-Hill, 1974.
15. YARNELL, J. L.; WARREN, J. L.; KOENING, S. H. Experimente! dispersion curves for phonons in aluminium. In: WALLIS, R. F. *Lattice dynamics: proceedings of the international conference held in Copenhagen Denmark, 5-9 Aug., 1963*. New York, Pergamon, 1963. p.247.
16. ZIMAN, J. M. *Principles of the theory of solids*. London, Cambridge, 1964.