

## Lattice dynamics of beryllium

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MS Received 15 January 1974

**Abstract.** Phonon frequencies in beryllium along the principal symmetry directions have been determined by means of the slow neutron inelastic scattering technique. The data are analysed in terms of a six-neighbour force constant model and the force constants are evaluated. It is concluded that strong tensor forces are present in beryllium and the importance of this finding to basic theories of lattice dynamics is pointed out.

**Keywords.** Lattice dynamics, phonons, beryllium, neutron scattering.

### 1. Introduction

This paper presents extensive measurements of phonon dispersion curves in beryllium along  $\Gamma A$ ,  $\Gamma M$ ,  $\Gamma KM$ , AL and AH directions using neutron spectrometry. The experiments were carried out on a filter-detector spectrometer (FDS) and a triple-axis spectrometer (TAS). Earlier measurements (Schmunk *et al* 1962, Schmunk 1966) were restricted mainly to  $\Gamma A$  and  $\Gamma M$  directions. In section 2 of this paper the experimental details are described and the results are presented in section 3. Some of these results have been reported earlier (Thaper *et al* 1971, Roy *et al* 1973). The analysis and discussion are given in section 4. The data are analysed in terms of a six-neighbour force constant model and the force constants are evaluated. On this basis it is shown that if one wants to arrive at a reasonable theoretical model to describe the lattice dynamics of hexagonal metals it is not sufficient to carry out measurements along  $\Gamma A$  and  $\Gamma M$  alone. From the measurements it is further concluded that strong tensor forces involving many body interactions are present in beryllium. Presence of such forces can be unequivocally proven by an examination of the sequence of frequencies at the point K in the Brillouin zone.

### 2. Experiment

#### 2.1 Sample

The experiments were performed on two different crystals. Crystal #1 was a slab of dimension 6.5 cm  $\times$  4.3 cm  $\times$  2.2 cm and most of the measurements on this were made on the TAS. Crystal #2 (7.1 cm  $\times$  3.8 cm  $\times$  1.4 cm) was utilised for most of the measurements on FDS. The quality of crystal #1 was

somewhat better than that of crystal #2 as judged from the measured shapes of some rocking curves. Therefore, some phonons were measured on both the spectrometers on the better crystal (#1), as a check on the accuracy of the measurements. In general, the measurements on the crystals #1 and #2 on the separate spectrometers gave fair agreement (Thaper *et al* 1971).

## 2.2 Measurements

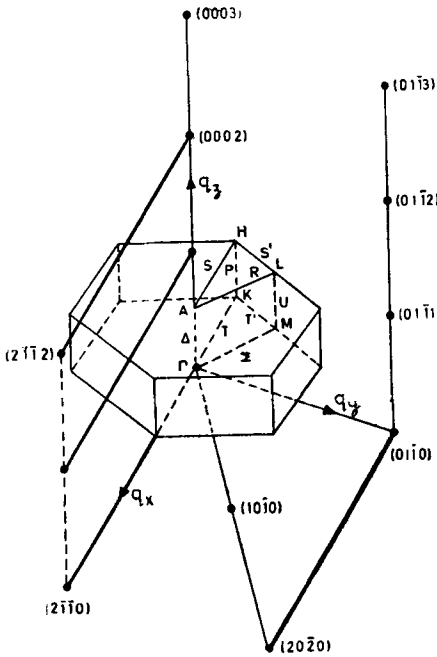
The FDS has not been used earlier in a systematic way to measure phonon frequencies. The reason for this mainly lies in the fact that a filter allows all neutrons above a certain wavelength to pass through, resulting in a poor resolution in the outgoing neutron wavevector  $k'$ . Further, unlike in a TAS where the analyser function is a Gaussian centered around the average outgoing wavevector, one has to deal here with an asymmetrical analyser function. Because of these reasons it has been believed rather erroneously that FDS cannot be used for accurate phonon work. It was therefore necessary to first justify that the FDS can indeed be used for such measurements. This was done in our laboratory recently both on experimental as well as theoretical basis and forms the subject of a separate paper (Thaper *et al* 1973). The main conclusions of this paper were the following :

(a) It is possible to measure phonon frequencies accurately using a FDS with a beryllium oxide filter, if one assumes the average outgoing energy  $E' = 2.5$  meV and average outgoing wavevector  $|k'| = 1.1 \text{ \AA}^{-1}$ . With these values of  $E'$  and  $k'$  the FDS can be used just like a TAS, even if the slopes of the phonon branches are fairly large. The intensities of the neutron groups (in the available regions of reciprocal space) measured using FDS are larger than in the conventional TAS.

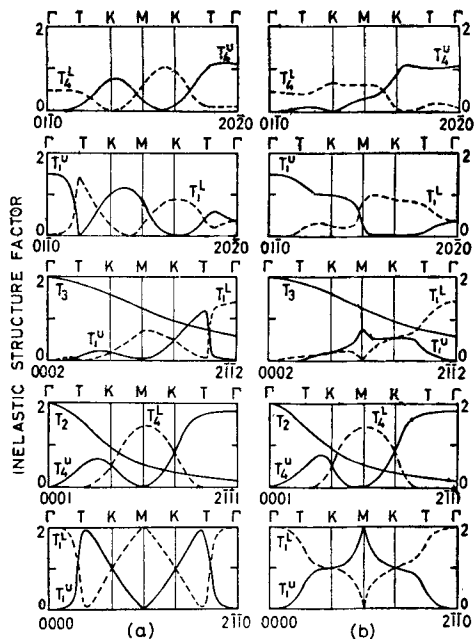
(b) Utilising the resolution formulae given earlier it is possible to predict the shapes of neutron groups theoretically with reasonable accuracy, and

(c) The FDS shows focusing properties similar to those of the TAS. It may be remarked here that a somewhat different method has been used by other workers (Haywood and Collins 1971, Bergsma 1970) to measure flat phonon branches.

The filter in the present measurements consisted of a combination of a block of beryllium oxide of size  $10 \text{ cm} \times 5 \text{ cm} \times 5 \text{ cm}$  preceded by beryllium made up of 6 slabs of size  $10 \text{ cm} \times 0.6 \text{ cm} \times 5 \text{ cm}$  each. The beryllium slabs faced the sample and were interleaved with cadmium to minimize the contribution of Bragg and multiply scattered neutrons. The spectrometer was mainly operated in the "constant- $Q$ " and "constant- $E$ " modes. With the energy and wavevector resolutions of the present experiments both the "constant- $Q$ " "constant- $E$ " modes of operation were unsatisfactory for some points. The phonons on  $\Delta_1$  and  $\Delta_2$  branches along  $\Gamma A$  for  $q/q_m$  between 0.9 and 1.0 were measured with the spectrometer programmed to scan along the normal to the dispersion curve. Table 1 lists the scattering planes and reciprocal lattice points (figure 1) around which data were collected for various phonon branches. Inelastic structure factors calculated by Schmunk *et al* (1962) were used as the guidelines for selecting the points for measurements along  $\Gamma A$  and  $\Gamma M$ . The structure factors for  $\Gamma KM$  were computed using the modified axially symmetric force constants given by DeWames *et al* (1965) and these are shown in figure 2 a.



**Figure 1.** Top half of the first Brillouin zone for a hexagonal lattice. The reciprocal lattice points around which measurements were made are also shown.



**Figure 2.** Inelastic structure factor calculations for the *TKM* branches along various lines (shown as thick lines in figure 1) in the reciprocal space using (a) the MAS model force constants given by DeWames *et al* (1965) and (b) the force constant model discussed in the text.

Some typical neutron groups and their calculated shapes are shown in figure 3 as illustrations. Details of focusing observed on the FDS can be found in the paper by Thaper *et al* (1973).

The measurements on the TAS were carried out in the “constant-*E*” mode of operation with fixed incoming energy  $E_0$ , which was chosen to be 0.09 eV except for some low energy transfer experiments where  $E_0$  was changed to 0.04 eV. The spectrometer was operated in the energy loss mode for the higher incident energy and in energy gain mode for the lower one. The reciprocal lattice points around which the measurements were made are included in table 1. Measurements of phonons with frequencies higher than 12 THz posed intensity problems. Therefore, such frequencies were measured using the FDS. Measurements along *TKM*, *AL* and *AH* were performed entirely on the FDS.

### 3. Results

The results of our measurements are given in figures 4–6 and the frequencies are tabulated in table 2. The labelling of the branches is given in accordance with standard group-theoretical notations (Warren 1968). The zone centre frequencies of 13.8 THz (459  $\text{cm}^{-1}$ ) and 20.1 THz (669  $\text{cm}^{-1}$ ) have been observed for the first time. The former frequency agrees very well with the one reported in recent Raman

Table 1. Choice of reciprocal lattice points for measuring various phonon branches

| Scattering plane | Branch index | Reciprocal lattice point                               | Scattering plane | Branch index | Reciprocal lattice point                               |
|------------------|--------------|--|------------------|--------------|--|
| $(q_y - q_z)$    | $\Delta_1$   | (0002), (01 $\bar{1}$ 2), (0004)*                      | $(q_x - q_y)$    | $\Sigma_4^v$ | (2 $\bar{1}\bar{1}$ 0)                                 |
|                  | $\Delta_2$   | (01 $\bar{1}$ 3)                                       |                  | $\Sigma_4^L$ | (10 $\bar{1}$ 0), (2 $\bar{1}\bar{1}$ 0)*              |
|                  | $\Delta_5$   | (01 $\bar{1}$ 1)                                       |                  | $T_1^L$      | (20 $\bar{2}$ 0)                                       |
|                  | $\Delta_6$   | (01 $\bar{1}$ 2), (02 $\bar{2}$ 1)*                    |                  | $T_4^v$      | (20 $\bar{2}$ 0)                                       |
|                  |              |  |                  | $T_4^L$      | (20 $\bar{2}$ 0)                                       |
|                  |              |  |                  |              |  |
|                  | $\Sigma_1^v$ | (01 $\bar{1}$ 2)                                       | $(q_x - q_z)$    | $T_1^v$      | (2 $\bar{1}\bar{1}$ 2)                                 |
|                  | $\Sigma_1^L$ | (01 $\bar{1}$ 2), (02 $\bar{2}$ 1)*, (01 $\bar{1}$ 0)* |                  | $T_1^L$      | (2 $\bar{1}\bar{1}$ 0)                                 |
|                  | $\Sigma_3^v$ | (0003)   |                  | $T_3$        | (2 $\bar{1}\bar{1}$ 1), (2 $\bar{1}\bar{1}$ 0), (0003) |
|                  | $\Sigma_3^L$ | (01 $\bar{1}$ 1), (0 $\bar{1}$ 13)*                    |                  | $T_3$        | (2 $\bar{1}\bar{1}$ 2)                                 |
|                  |              |  |                  |              |  |

\* Measurements made in a triple-axis spectrometer. The rest refer to the filter-detector spectrometer.

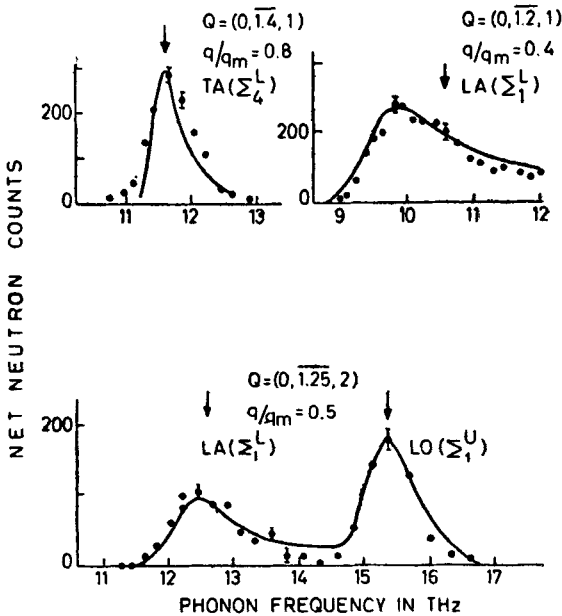


Figure 3. Some typical examples of phonons observed in beryllium using the filter-detector spectrometer. Solid lines are the calculated shapes of neutron groups.

scattering measurements ( $455 \text{ cm}^{-1}$ ) (Feldman *et al* 1968). The dispersion curves show a general qualitative agreement with the measurements of Schmunk (1966); the present data however, show less scatter. A quantitative comparison between the two shows differences along the  $\Delta_1$ ,  $\Delta_5$  and  $\Sigma_1^v$  branches.

#### 4. Analysis

##### 4.1 Force constant models

It is not uncommon to analyse the measured phonon dispersion curves in hcp metals in terms of modified axially symmetric (MAS) model by fitting the calculations

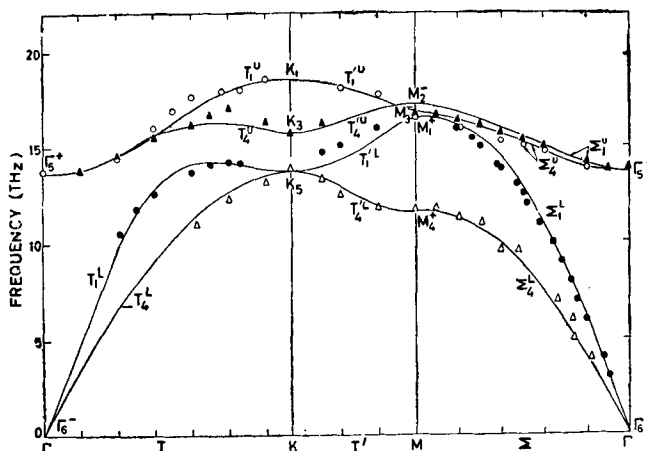


Figure 4. Phonon dispersion data along  $\Gamma$ KM and  $\Gamma$ M for the modes polarized in the basal plane. The solid lines represent a six-neighbour force constant model fit to the data along  $\Gamma$ A,  $\Gamma$ M and  $\Gamma$ KM. The model includes tensor force interactions for the nearest neighbours in the basal plane and modified axially-symmetric interactions for the remaining neighbours.

to data along  $\Gamma$ A and  $\Gamma$ M directions. (See for example, DeWames *et al* 1965, Sinha *et al* 1970, Wakabayashi *et al* 1971, Upadhyaya and Verma 1973). This was initially tried when our measurements along  $\Gamma$ A and  $\Gamma$ M were complete. However, attempts to obtain a non-linear least square fit to the data along these directions within the framework of the six-neighbour MAS model with 17 parameters led to convergence difficulties. Similar difficulties have been reported in literature earlier also (Sinha *et al* 1970). This difficulty could arise either because the model is unrealistic or because sufficient orthogonal information is not available to fit all the parameters of the model. In order to investigate this point the measurements were extended to  $\Gamma$ KM, AH and AL directions as reported in section 3. Fits using the MAS model, with the additional data included, did not give any convergence problems, thus clearly showing that measurements along a direction other than  $\Gamma$ A and  $\Gamma$ M is necessary to describe the lattice dynamics properly. Though there were no convergence problems the fit itself was not satisfactory around the point K. The best fit obtained is shown in figure 7 with dashed lines. In

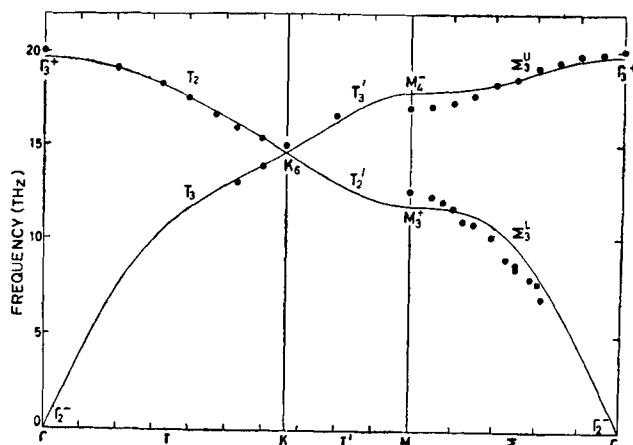


Figure 5. Phonon frequencies along  $\Gamma$ K and  $\Gamma$ M for the modes polarized perpendicular to the basal plane. The solid lines have the same meaning as in figure 4.

**Table 2.** Phonon frequencies<sup>+</sup> of Be at 297 K in THz. Notations as in figure 1.

| $q_x$ | $T_1^v, T_1'^v$ | $q_x$  | $T_4^L, T_4'^L$   | $q_y$ | $\Sigma_3^L$              | $q_x$ | $\Delta_1$ |
|-------|-----------------|--------|---|-------|---------------------------|-------|------------|
| 0.20  | 14.45           | 0.42   | 11.00   | 0.38  | 7.00*                     | 0.31  | 6.05       |
| 0.30  | 16.00           | 0.50   | 12.25   | 0.40  | 7.75                      | 0.36  | 7.00*      |
| 0.35  | 16.90           | 0.60   | 13.20   | 0.43  | 8.00*                     | 0.41  | 8.05       |
| 0.40  | 17.65           | 0.67   | 14.00   | 0.50  | 8.50*                     | 0.48  | 8.80*      |
| 0.48  | 17.95           | 0.75   | 13.35   | 0.50  | 8.78                      | 0.51  | 9.15       |
| 0.53  | 18.05           | 0.80   | 12.50   | 0.55  | 9.00*                     | 0.52  | 9.00*      |
| 0.60  | 18.60           | 0.90   | 11.85   | 0.62  | 10.25                     | 0.56  | 9.87*      |
| 0.80  | 18.10           | 1.00   | 11.75   | 0.65  | 10.00*                    | 0.58  | 10.15      |
| 0.90  | 17.75           |        |   | 0.70  | 10.82                     | 0.61  | 10.15      |
|       |                 |        |   | 0.75  | 11.00*                    | 0.63  | 11.00*     |
|       |                 |        |   | 0.80  | 11.70                     | 0.64  | 10.75*     |
|       |                 |        |   | 0.85  | 12.00*                    | 0.72  | 11.30      |
|       |                 |        |   | 0.90  | 12.30                     | 0.74  | 11.80*     |
|       |                 |        |   | 1.00  | 12.60                     | 0.75  | 12.00*     |
|       |                 |        |   |       |                           | 0.82  | 12.05      |
|       |                 |        |   |       |                           | 0.82  | 12.70*     |
|       |                 |        |   |       |                           | 0.84  | 13.00*     |
|       |                 |        |   |       |                           | 0.86  | 13.10      |
|       |                 |        |   |       |                           | 0.90  | 13.80      |
|       |                 |        |   |       |                           | 0.96  | 14.15      |
| $q_x$ | $T_1^L, T_1'^L$ | $q_y$  | $\Sigma_1^v$  | $q_y$ | $\Sigma_4^v$              |       |            |
| 0.20  | 10.50           | 0.10   | 13.87   | 0.00  | 13.85                     |       |            |
| 0.25  | 11.75           | 0.20   | 14.25   | 0.20  | 13.90                     |       |            |
| 0.30  | 12.55           | 0.40   | 15.05   | 0.40  | 14.75                     |       |            |
| 0.40  | 13.70           | 0.50   | 15.40   | 0.50  | 15.07                     |       |            |
| 0.45  | 14.10           | 0.60   | 15.82   | 0.60  | 15.30                     |       |            |
| 0.50  | 14.20           | 0.70   | 16.25   | 0.80  | 16.00                     |       |            |
| 0.53  | 14.15           | 0.80   | 16.47   | 1.00  | 16.60                     |       |            |
| 0.75  | 14.70           | 0.90   | 16.75   |       |                           |       |            |
| 0.80  | 15.05           | 1.00   | 16.82   |       |                           |       |            |
| 0.90  | 16.00           |        |   |       |                           |       |            |
| $q_x$ | $T_2, T_2'$     | $q_y$  | $\Sigma_1^L$  | $q_z$ | $\Delta_2$                |       |            |
| 0.20  | 19.20           | 0.09   | 3.00*   | 0.00  | 20.10                     |       |            |
| 0.33  | 18.35           | 0.12   | 4.00*   | 0.10  | 20.10                     |       |            |
| 0.40  | 17.55           | 0.20   | 6.00*   | 0.20  | 19.87                     |       |            |
| 0.47  | 16.70           | 0.24   | 7.00*   | 0.30  | 19.80                     |       |            |
| 0.53  | 15.90           | 0.28   | 8.00*   | 0.40  | 18.85                     |       |            |
| 0.60  | 15.35           | 0.32   | 9.00*   | 0.50  | 18.45                     |       |            |
|       |                 | 0.36   | 10.00*  | 0.60  | 17.85                     |       |            |
|       |                 | 0.42   | 11.00*  | 0.70  | 17.25                     |       |            |
|       |                 | 0.48   | 12.00*  | 0.80  | 16.70                     |       |            |
|       |                 | 0.50   | 12.55   | 0.83  | 16.65                     |       |            |
|       |                 | 0.53   | 13.00*  | 0.90  | 16.00                     |       |            |
| $q_x$ | $T_3, T_3'$     | $0.60$ | 13.82 <th>0.96</th> <th>15.35 <th></th> <th></th> </th> | 0.96  | 15.35 <th></th> <th></th> |       |            |
| 0.53  | 13.00           | 0.62   | 14.00*  | 0.98  | 15.25                     |       |            |
| 0.60  | 13.90           | 0.70   | 15.03   | 1.00  | 15.00                     |       |            |
| 0.67  | 15.00           | 0.74   | 15.40   |       |                           |       |            |
| 0.80  | 16.60           | 0.81   | 16.00   |       |                           |       |            |
| $q_x$ | $T_4^v, T_4'^v$ | $q_y$  | $\Sigma_3^v$  | $q_z$ | $\Delta_5$                |       |            |
| 0.10  | 13.80           | 0.10   | 19.92   | 0.00  | 13.75                     |       |            |
| 0.20  | 14.60           | 0.20   | 19.80   | 0.10  | 13.75                     |       |            |
| 0.30  | 15.50           | 0.30   | 19.52   | 0.20  | 13.62                     |       |            |
| 0.40  | 16.20           | 0.40   | 19.17   | 0.30  | 13.55                     |       |            |
| 0.45  | 16.70           | 0.50   | 18.55   | 0.40  | 13.33                     |       |            |
| 0.50  | 17.05           | 0.60   | 18.25   | 0.50  | 13.12                     |       |            |
| 0.60  | 16.35           | 0.70   | 17.65   | 0.60  | 12.65                     |       |            |
| 0.67  | 15.80           | 0.80   | 17.32   | 0.70  | 12.25                     |       |            |
| 0.75  | 16.30           | 0.90   | 17.07   | 0.80  | 11.90                     |       |            |
|       |                 | 1.00   | 17.00   | 0.90  | 11.45                     |       |            |
|       |                 |        |   | 1.00  | 10.75                     |       |            |
| $q_x$ |                 | $q_y$  |   | $q_z$ | $\Delta_6$                |       |            |
|       |                 |        |   | 0.36  | 5.00*                     |       |            |
|       |                 |        |   | 0.42  | 5.70*                     |       |            |
|       |                 |        |   | 0.54  | 7.00*                     |       |            |
|       |                 |        |   | 0.63  | 7.70*                     |       |            |
|       |                 |        |   | 0.70  | 8.85                      |       |            |
|       |                 |        |   | 0.80  | 9.65                      |       |            |
|       |                 |        |   | 0.87  | 10.15                     |       |            |

$q_x, q_y$  and  $q_z$  are expressed in units of  $(2\pi/a)$ ,  $(2\pi/\sqrt{3}a)$  and  $(\pi/c)$  respectively.

<sup>+</sup> Based on counting statistics and the shapes of neutrons groups, the errors on the frequencies vary from 1-3%.

\* Measurements made in a triple-axis spectrometer. The rest of the measurements were carried out using the filter-detector spectrometer.

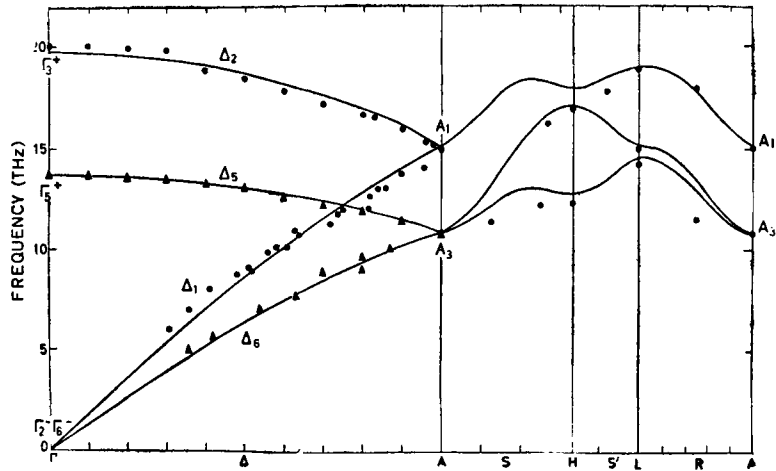


Figure 6. Phonon frequencies along  $\Gamma A$  and on the surface of the Brillouin zone along  $AH$  and  $AL$ . The solid lines have the same meaning as in figure 4.

particular, it was found that within the framework of MAS model it was impossible to reproduce the observed sequence of  $T_1$  and  $T_4$  branches at the point  $K$  (see figures 4 and 7). Irrespective of the number of neighbours taken into consideration one always obtains a doubly degenerate branch between two non-degenerate ones. The reason for this can be readily seen by writing the general expression for the frequencies at  $K$ :

$$\begin{aligned} \nu_{K_5}^2 &= \frac{1}{4\pi^2 M} [D_{xx}(q, 11) + \text{Im}D_{xy}(q, 11)] \quad \text{Doubly Degenerate} \\ \nu_{K_1}^2 &= \frac{1}{4\pi^2 M} [D_{xx}(q, 11) + 2\text{Re}D_{xx}(q, 12) - \text{Im}D_{xy}(q, 11)] \\ \nu_{K_3}^2 &= \frac{1}{4\pi^2 M} [D_{xx}(q, 11) - 2\text{Re}D_{xx}(q, 12) - \text{Im}D_{xy}(q, 11)]. \end{aligned} \quad (4.1)$$

In the MAS model  $\text{Im}D_{xy}(q, 11)$  is identically zero and one therefore gets  $|\nu_{K_1}^2 - \nu_{K_5}^2| = |\nu_{K_3}^2 - \nu_{K_5}^2|$ . In other words the doubly degenerate branch lies exactly in the middle of two non-degenerate ones. In tensor force models, since  $\text{Im}D_{xy}(q, 11) \neq 0$  different ordering is possible. For example, one may also have  $\nu_{K_1}$  and  $\nu_{K_3} > \nu_{K_5}$  or  $\nu_{K_1}$  and  $\nu_{K_3} > \nu_{K_5}$ . In Be one finds that  $\nu_{K_1} > \nu_{K_3} > \nu_{K_5}$  which shows that the MAS model is inherently inadequate for describing the dynamics. As an alternative of the MAS model, mention may be made of the work of Srinivasan and Ramji Rao (1971) who have explicitly taken into account three-body forces following Keating's approach, in addition to two-body forces. But  $D_{xy}(q, 11)$  is still real in this model.

To make the model consistent with the present observations tensor force interaction for the nearest neighbours in the basal plane was included. Based on such a model (hereafter called the TF model) with just one more parameter than the earlier MAS model, a new set of force constants was obtained by a non-linear least square fit to the data along  $\Gamma A$ ,  $\Gamma M$  and  $\Gamma K$  and the elastic constants. Again

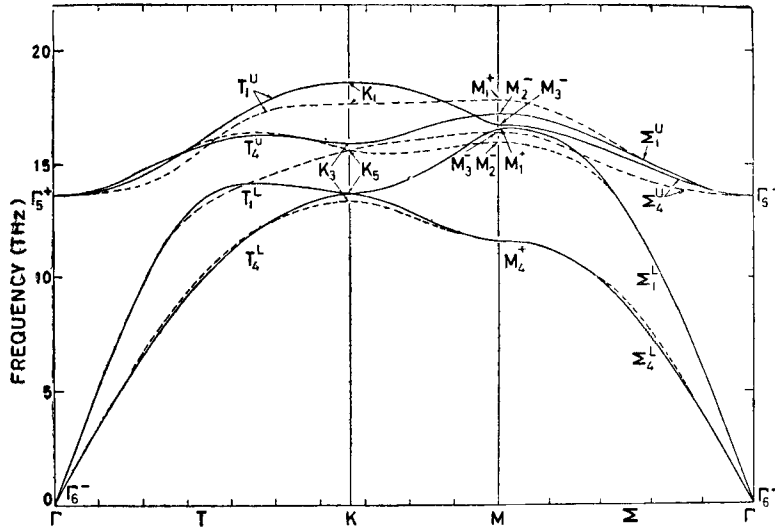


Figure 7. The dashed lines show the six-neighbour MAS model fit to the present data. The solid lines have the same meaning as in figure 4. Note in particular the difference in ordering of the branches in the two models at K and interchange of labelling at M. (--- MAS ; — TF)

no convergence problem was encountered. The fitted force constants and the calculated elastic constants are given in table 3 and the dispersion curves along the various directions are shown in figures 4 to 6, with continuous lines, as also in figure 7 for comparison with the MAS model results.

Since the MAS model is not adequate for describing the lattice dynamics, especially along  $\Gamma K$ , it was thought that it may be worthwhile examining the inelastic structure factor based on the TF model. This was done for some of the branches along  $\Gamma K$  and is given in figure 2b. These have to be compared with the structure factors calculated using the MAS model and shown in figure 2a. Along the line  $(0000) \rightarrow (2\bar{1}\bar{1}0)$  the MAS model predicts an abrupt change in the structure factor which arises from a sudden interchange of polarisation vectors between  $T_1^U$  and  $T_1^L$  branches at  $q = 0.33 (2\pi/a)$ . This change-over is absent in the TF model. There is also a change-over in the structure factors at the point M along the same line; this, however, is merely a consequence of interchange of labelling of the branches (see figure 7 for labelling). Measurements of the intensities of these phonons would provide further evidence for the validity of the TF model. However, since the phonon frequency measurements along  $\Gamma K$  were carried out on the FDS, which has a restricted coverage in the reciprocal space, a systematic investigation of the intensity of neutron groups around regions of interest was not feasible.

#### 4.2 Basic Calculations

Several microscopic calculations of the dispersion curves of hcp metals have been carried out based on the pseudopotential theory (King and Cutler 1970, and the references cited therein). King and Cutler (1970) obtain good agreement with experimental results along  $\Gamma A$  and  $\Gamma M$  in beryllium, using what the authors call a non-local pseudopotential approach. But in all these calculations which employ second order perturbation theory in the pseudopotential starting with plane waves the electronic contribution to the dynamical matrix  $D_{\mathbf{x}\mathbf{x}'}(\mathbf{q}, 11)$  can be expressed as



Table 3a. Best fit six-neighbour force model for beryllium.

| Neighbour | Force constant  | dyne/cm. | Neighbour | Force constant          | dyne/cm. |
|-----------|-----------------|----------|-----------|-------------------------|----------|
| 1         | $\delta_1$      | 2132     | 4         | $\beta_{4x}$            | 3605     |
|           | $\epsilon_{1y}$ | 3678     |           | $\alpha_4 + \beta_{4z}$ | 5358     |
|           | $\epsilon_{1z}$ | 1878     |           |                         |          |
| 2         | $\alpha_2$      | 13285    | 5         | $\delta_5$              | 53       |
|           | $\beta_{2x}$    | 3265     |           | $\epsilon_{5y}$         | 230      |
|           | $\beta_{2z}$    | 1105     |           | $\epsilon_{5z}$         | 1306     |
|           | $\delta^*$      | -6223    |           |                         |          |
| 3         | $\delta_3$      | 220      | 6         | $\alpha_6$              | 1639     |
|           | $\epsilon_{3x}$ | -2534    |           | $\beta_{6x}$            | 688      |
|           | $\epsilon_{3z}$ | -3416    |           | $\beta_{6z}$            | 1292     |

\* For the definition of the tensor force constant  $\delta$  see Iyengar *et al* (1965). The remaining MAS model force constants are defined following DeWames *et al* (1965).

Table 3b. Comparison of calculated and experimental elastic constants for beryllium (in units of  $10^{11}$  dyne/cm<sup>2</sup>).

| Elastic Constant | Experimental <sup>a</sup> | Calculated  | Elastic Constant | Experimental | Calculated |
|------------------|---------------------------|---|------------------|--------------|------------|
| $C_{11}$         | 29.23                     | 27.62   | $C_{66}$         | 13.28        | 11.85      |
| $C_{33}$         | 33.64                     | 31.31   | $C_{13}$         | 1.40         | 1.29       |
| $C_{44}$         | 16.25                     | $\left. \begin{array}{l} 15.83^b \\ 16.53^c \end{array} \right\}$ |                  |              |            |

<sup>a</sup> Smith and Arbogast (1960).

<sup>b</sup> Calculated from the expression of  $C_{44}$  as obtained by taking the limiting slope ( $q \rightarrow 0$ ) along  $\Gamma M$ .

<sup>c</sup> From the limiting slope along  $\Gamma A$ . It may be noted that the condition of rotational invariance leads to the identity of above two expressions for  $C_{44}$ .

$$D_{xy}^F(\mathbf{q}, 11) = \text{const.} \sum_{\tau} [(\tau + \mathbf{q})_x (\tau + \mathbf{q})_y E(|\tau + \mathbf{q}|) - (\tau)_x (\tau)_y (1 + \cos \tau \cdot \mathbf{r}_{12}) E(|\tau|)] \quad (4.2)$$

where  $\mathbf{r}_{12}$  is the separation of the atoms 1 and 2 in the unit cell,  $\tau$  is a reciprocal lattice vector and  $E(|\mathbf{Q}|)$  is Harrison's energy-wavenumber characteristics which is real. Therefore  $D_{xy}^F(\mathbf{q}, 11)$  is real and the same is true for  $D_{xy}^C(\mathbf{q}, 11)$ , arising from the direct coulomb interaction between the ions. Thus,  $\text{Im} D_{xy}(\mathbf{q}, 11)$  is zero as in the MAS model. It may be stated in general that any calculation which involves pairwise interactions between the particles, irrespective of whether it is based on a force constant model or pseudopotential theory, predicts a degenerate frequency  $\nu = (D_{xx}(\mathbf{q}, 11)/4\pi^2 M)^{1/2}$  (see equation 4.1) at K, with one non-degenerate frequency higher and another lower, contrary to the observation in some hcp substances.

Bertoni *et al* (1973) have recently reported a first principle calculation of the lattice dynamics of beryllium where the total electron energy up to the third order in the electron-ion pseudopotential has been considered and its explicit contribution to the dynamical matrix has been evaluated. The authors find that this scheme, which in effect gives rise to three body forces, leads to the correct sequence of the branches at K, apart from improving the overall agreement with experiments.

## 5. Summary

Detailed measurements of phonon dispersion curves in Be along  $\Gamma A$ ,  $\Gamma M$ ,  $\Gamma KM$ , AL and AH are reported. Force constants based on a six neighbour model, described in the text, are evaluated. It is shown that in hcp metals it is necessary to make measurements along directions other than  $\Gamma A$  and  $\Gamma M$  in order to evaluate realistic force constants. The sequence of branches at the point K is shown to throw light on the nature of forces in hcp substances. In particular, in beryllium they prove the existence of strong tensor forces. Ordering similar to that in beryllium is found in many other hcp metals (Roy *et al* 1973). The importance of this finding in relation to basic theories of lattice dynamics is pointed out.

## Acknowledgements

We thank V C Sahni, S K Sinha and G Venkataraman for valuable discussions, V Bortolani for sending the results of his calculation prior to publication and P R Vijayaraghavan for non-linear least square fitting programme. We gratefully acknowledge the technical assistance given by T Srinivasan.

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