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CALCULATION OF PHONON DISPERSION CURVES AND DENSITY OF STATES: USE OF SIMPLE PROGRAM WITH PERSONAL COMPUTERS

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ABSTRACT

The phonon density of state and dispersion relation of one and two atoms crystal structures have been evaluated for simple cubic and body centered lattices with interatomic interactions upto and including second neighbours. The force constants in simple structures are determined by an optimization procedure using the dispersion in the [100], [110] and [111] directions. The dispersion curves calculated with a two neighbours, six parameter give a reasonable fit to the dispersion data in the principal sysmmetry directions.

The standard FORTRAN code available in the literature has been substantially modified for adaptation for personal computer. All the needed subroutines are suitably modified to create a versatile program which can be used for any lattice phonon dispersion and density of states calculations.

1. INTRODUCTION

The solution of numerical problems in theoretical physics used to be the domain of large computers. However, in recent years there have appeared on the market personal computers which are as powerful as the computers of the early sixties. Apart from their computational performance, personal computers offer graphical output of results, which were not available twenty years ago. Personal computers accordingly offer us a wide field of possibilities in education and research.

The advantage of the p.c. in solving any problem is that one can easily vary the physical parameters and the boundary conditions or the initial conditions interactively and so become familiar with a whole family of solutions. The quantized normal modes of vibration of the crystal lattice with energy $h\omega$, are called phonons. Knowledge of Phonon dispersion relation and density of states is useful in the study of the thermal and optical properties of solids. In this article, we present the solution of phonon dispersions and densities of states for simple cubic and body cubic centered lattices. This problem was solved long ago (e.g, see Keeler, 1980) using large computers in so called Time - Sharing mode. We have modified his Computer code in the Boardman series book, from a version of FORTRAN 66 written for the Mainframe Computers, to the Microsoft FORTRAN 77 version for Personal Computers. We also substitute the *Numerical Algorithm Group's*

(NAG) subroutine F02AAF called in the original program by one found in Curtis (1989).

2. THE DYNAMICAL MATRICES FOR SC AND BCC LATTICES

The classical model of the vibrating lattices consists of a number of atoms, of point masses m, forming linear chains. The most important quantities in lattice dynamics are the second order coupling (force) constants:

$$\Phi_{ll'} = \frac{\partial^2 U}{\partial u_l \partial u_{l'}} \tag{1}$$

Where U is the total potential of the syatem and u_l and $u_{l'}$ are the displacement of atoms l and l' in the chain, respectively. The equation of motion of a mass at the origin, 0, due to displacement of atom u_l is

$$F_0 = m\frac{\partial^2}{\partial t^2}u_{0,\alpha} = -\sum_l \sum_{\beta=1}^{3} \Phi_{l,\alpha\beta} u_{l,\beta} \tag{2}$$

where α and β represent the cartesian components, x, y and z. We let

$$u_{l,\alpha}(\vec{k}) = A_\alpha \exp[i(\omega t - \vec{k}.\vec{r}_l\,) \tag{3}$$

and define

$$B_\alpha = \sqrt{m}A_\alpha \tag{4}$$

$$D_{\alpha\beta} = m^{-1}\sum \Phi_{l,\alpha\beta} \exp(i\vec{k}.\vec{r}_l\,) \tag{5}$$

On substitution of these in equation (2), we obtain

$$\omega^2 B_\alpha = \sum_{\beta=1}^{3} D_{\alpha\beta} B_\beta \qquad \alpha = 1, 2, 3 \tag{6}$$

or

$$\omega\vec{B} = D(\vec{k}).\vec{B} \tag{7}$$

The matrix $D(\vec{k}\,)$ is called the dynamical matrix for one atom unit cell. The resulting secular equation

$$|D(\vec{k}\,) - \omega^2\delta_{ij} = 0 \tag{8}$$

has roots $\omega^2(\vec{k}\,)$ which are the eigenvalues of $D(\vec{k}\,)$.

The dynamical matrix for a lattice with basis of n atoms has 3n x 3n dimensions and here also,

$$\omega^2\vec{B} = D'(\vec{k}).\vec{B} \tag{9}$$

The dynamical matrix for two-atom unit cells can be partioned into 2^2 submatrices

$$D'(\vec{k}) = \begin{pmatrix} D(\vec{k},11) D(\vec{k},12) \\ D(\vec{k},21) D(\vec{k},22) \end{pmatrix} \tag{10}$$

each of which is of order 3.

Four unit cells of single atoms simple cubic lattice, with lattice constants a,; the radial directions $\vec{r}_l = \vec{a}\vec{\ell}$, $l = (l_1, l_2, l_3)$, where l_1, l_2, and l_3 are either all odd or all even integers are shown in figure 1. The nearest neighbour atoms 1 to 6 have the [100] type directions. They contribute a unit displacement of atom 0 in the x, y and z directions. Therefore

$$-\Phi_{1,xx} = -\Phi_{2,zz} = -\Phi_{3,yy} = -\Phi_{4,xx} = -\Phi_{5,zz} = -\Phi_{6,yy} = \gamma \qquad (11)$$

where γ is the force constant. The second nearest neighbors, atoms 7 to 18, have the [110] type directions and thier contributions to Φ are calculated as

$$-\Phi_7 = -\Phi_9 = {}^{R\gamma}\!/_2 \begin{pmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, -\Phi_8 = -\Phi_{10} = {}^{R\gamma}\!/_2 \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$(12)$$

$$-\Phi_{11} = -\Phi_{13} = {}^{R\gamma}\!/_2 \begin{pmatrix} 1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}, -\Phi_{12} = -\Phi_{14} = {}^{R\gamma}\!/_2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

$$-\Phi_{15} = -\Phi_{17} = {}^{R\gamma}\!/_2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \end{pmatrix}, -\Phi_{16} = -\Phi_{18} = {}^{R\gamma}\!/_2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

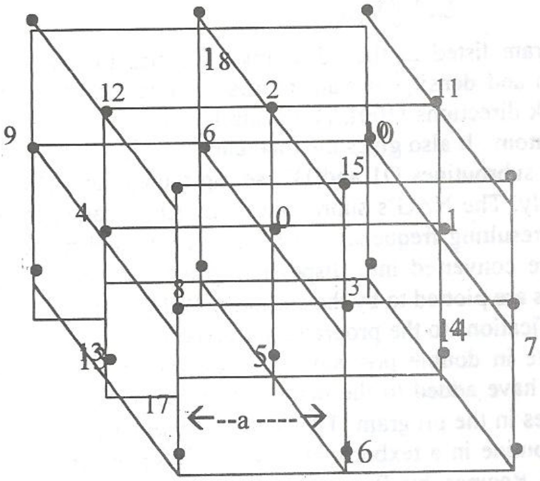

Fig.1. The SC lattice showing four unit cells and up to two nearest neighbor atoms atom 0 at the center.

Finally, the force on atom 0 due unit displacement of itself is obtaned from :

$$-\Phi_0 = -2\ (\gamma + 6R) \tag{13}$$

Combining equations (11), (12) and (13) and making use of the dynamical matrix for a one-atom simple cubic lattice , we obtain

$$D(\vec{k}) = \frac{2\gamma}{m}\begin{pmatrix} \Delta + RC_Y C_Z - C_X & S_X S_Y & S_X S_Z \\ S_X S_Y & \Delta + RC_X C_Z - C_Y & S_Y S_Z \\ S_X S_Z & S_Y S_Z & \Delta + RC_X C_Y - C_Z \end{pmatrix} \tag{14}$$

where $C_X = \cos k_x a$, $S_X = \sin k_x a$, $C_{2X} = \cos 2k_x a$ and $\Delta = 1 + [3 - (C_X C_Y + C_X C_Z + C_Y C_Z)]R$. The one- and two–atom the dynamical matrices have been calculated (Boardman 1981) and for the one-atom is

$$D(k) = \frac{8\gamma}{3m}\begin{pmatrix} \delta - \tfrac{3}{4} RC_{2X} & S_X S_Y C_Z & S_X C_Y S_Z \\ S_X S_Y C_Z & \delta - \tfrac{3}{4} RC_{2Y} & C_X S_Y S_Z \\ S_X C_Y S_Z & C_X S_Y S_Z & \delta - \tfrac{3}{4} RC_{2Z} \end{pmatrix} \tag{15}$$

where $\delta = 1 + 0.75R - C_X C_Y C_Z$.

3. THE COMPUTER PROGRAMMING

Analytical calculations of dispersion curves are performed by solving the secular determinant . This may not be feasible for two atoms per unit cells, and above, because of high order polynomials involved (Oh and Kok 1997). The density of states in three dimensions also require performing a difficult integration over a constant surface S (Animalu 1981):

$$G(\omega) = \frac{1}{8\pi^3}\int_S \frac{1}{\vec{\nabla}_k \omega} d\omega$$

The program listed in the "Boardman Physics Program" book compute and plots the dispersion and density of state curves for one- and two- atoms unit cells for the three principal k directions [100], [110] and [111]. It also give the total curves of each of the two case atom . It also gives the total curves for each case.

The main subroutines D1 and D2, set up the dynamical matrices of one and two atoms respectively. The NAG's subroutine F02AAF is called to solve the eigenvalue equation (9). The resulting frequencies of the three normal modes and the corresponding wave vectors are converted into dispersion graphs by the subroutine PRDC and the stored histograms are plotted to by the suroutine PRDOS.

The modifications to the program, are given in the appendix. The program is reformatted to calculate in double precision to make the errors resulting from the small numbers which we have added to the matrix elements in D1 and D2, and to eliminate all other singularities in the program. The NAG subroutine F02AAF has been subsituted with the PQR subroutine in a texbook by Curtis (1989). A similar subroutine, QR, found in the Numerical Recipes by Press et. al (1992) fails simetimes, after several runs. The subroutines PRDC and PRDOS are modified by adding the Fortran WRITE statement to produce numbers for plotting with a suitable graphing software. Some sample graphs have been presented. The input data were supplied interactively, and they are: ATOMS (number of atoms, 1 or 2), R (the ratio of second to first nearest neighbour force constants, between 0 and 1), RO (the ratio of m_1 and m_2 in case of two-atom cells) and INT (between 10 and 50, used for calculating the density of states).

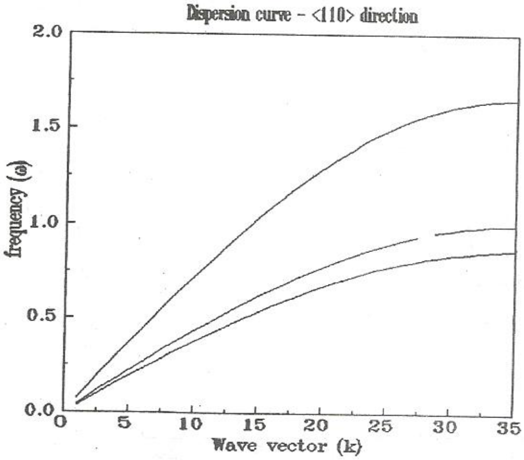

Figure (2). The [110] phonon dispersion curve for a monatomic SC crystal lattice. Force constant ratio R = .5

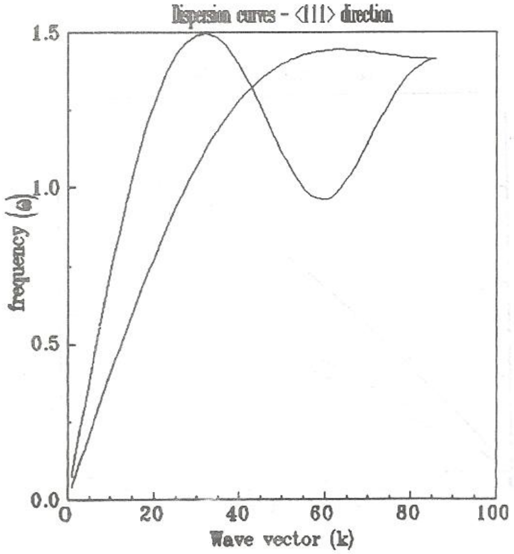

Figure (3). The [111] phonon dispersion curve for a monatomic BCC crystal lattice. Force constants ratio R = .5.

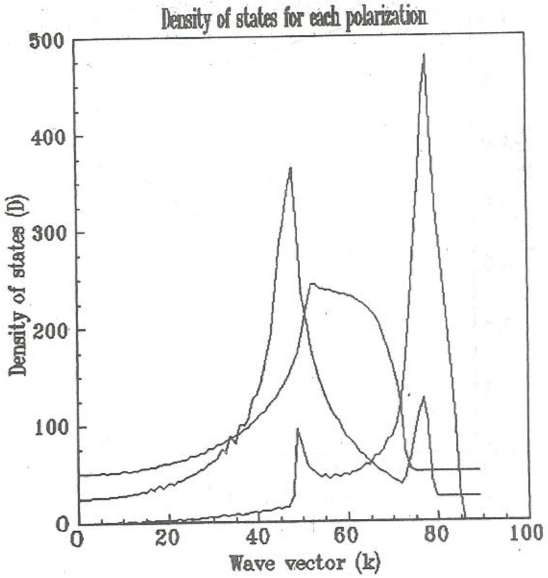

Fig. * The phonon density of states for each polarizations for one-atom BCC, **R=.5**

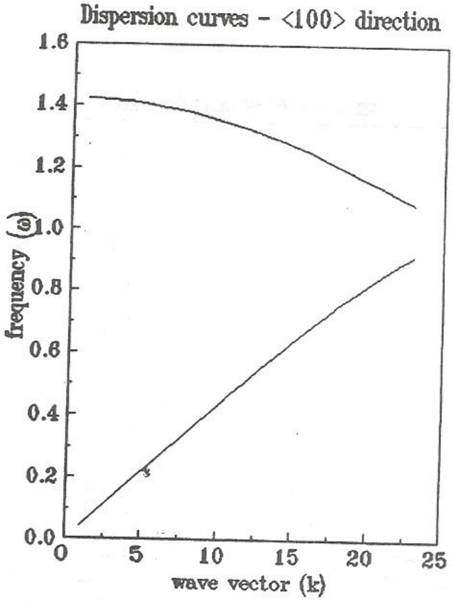

Fig. (A III). The phonon total density of states. This particular curve is for a one atom SC lattice with R = .5

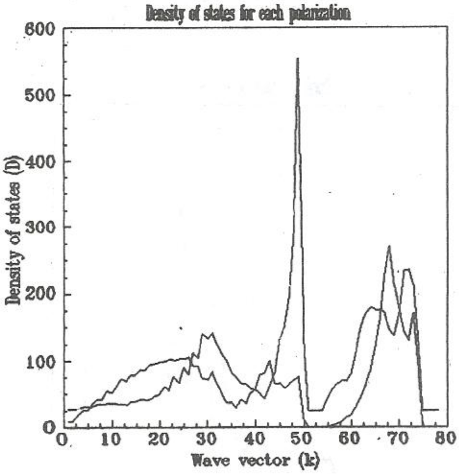

Fig.9 The phonon density of states for each polarizations. This perticular curves are for mass ratio p = .8 and force constant ratio r = 0.0

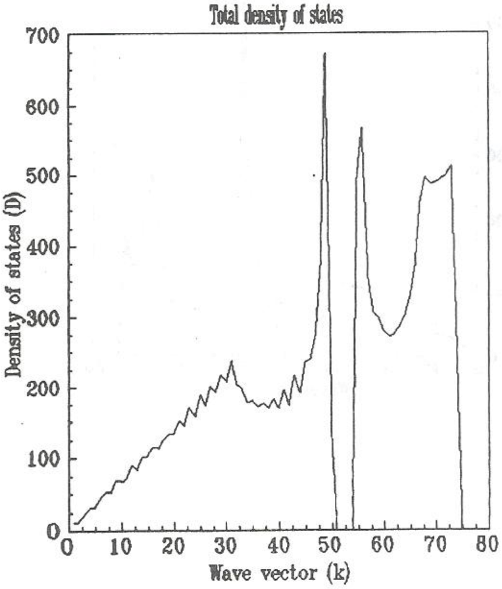

Fig. 10 The phonon total density of states. This particular curve is for mass ratio p = .8 and force constant ratio r =0.0.

5. CONCLUSIONS

The knowledge of dispersion curves and density of states is indispensable in the study of physical properties of crystalline solids. However, these quantities can only be determined numerically. A good computer program has been written and can be found in a graduate textbook, (Boardman ed. 1980). Unfortunately, this program was written in Fortran 66 Language and designed for the mainframe computers and it requires an external subroutine, from the NAG's library. All these are not easily available in this part of the world. Therefore, we undertook to modify the program to Fortran 77 for use on the personal computers (PC) and we substituted the external program with an internal and more suitable subroutine. Sample calculations were performed and presented for the SC and the BCC lattices.

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APPENDIX

```
      SUBROUTINE D1(DIR,K,QX,QY,QZ,R,W,IFAIL)
   INTEGER DIR,K,I,J,IFAIL
   double precision QX,QY,QZ,R,DIAG,D(12,10),S(3),C(3),W2(3),
  + W(3,6,200)
   C(1)=dCOS(QX)
   C(2)=dCOS(QY)
   C(3)=dCOS(QZ)
   S(1)=dSIN(QX)
   S(2)=dSIN(QY)
   S(3)=dSIN(QZ)
   DIAG=1.d0+((3-(C(1)*C(2)*C(3))*R)
   D(1,1)=DIAG+R*C(2)*C(3)-DCOS(2.0*QX) +.000000111
   D(2,2)=DIAG+R*(C1)*C(3)-DCOS(2.0*QY).+00000000111
   D(3,3)=DIAG+R*(C1)*C(3)-DCOS(2.0*QZ)
   D(1,2)=S(1)*S(2)+.0000001231
   D(2,3)=S(2)*S(3)
   D(3,1)=S(1)*S(3)+.0000000135
   D(2,1)=D(1,2)+.000000011234
   D(3,2)=D(2,3)
   D(1,3)=D(3,1)
   DATA (D(I,1),I=4,12)/9*0 /
   DATA (D(I,2),I=4,12)/ 9*0/
   DATA (D(I,3),I=4,12)/ 9*0/
   DATA ((D(I,J),I=1,12),J=4,10) /84*0 /


     SUBROUTINE D2(DIR,K,QX,QY,QZ,R,RO,W,IFAIL)
   INTEGER DIR,K,I,J,IFAIL
   double precision QX,QY,QZ,R,RO,ROOTRO,D(20,20),S(3),C(3),W2(6),
  + W(3,6,200)
   C(1)=dCOS(QX)
   C(2)=dCOS(QY)
   C(3)=dCOS(QZ)
   S(1)=dSIN(QX)
   S(2)=dSIN(QY)
   S(3)=dSIN(QZ)
   ROOTRO=dSQRT(RO)
   DO 801 I=1,6,1
     DO 801 J=1,6,1
     D(I,J)=0.0d0
801 CONTINUE
```

```
   D(1,1)=ROOTRO*(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QX))
   D(2,2)=ROOTRO*(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QY))
   D(3,3)=ROOTRO*(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QZ))
   D(4,4)=(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QX))/ROOTRO
   D(5,5)=(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QY))/ROOTRO
   D(6,6)=(1.0+0.75d0*R-0.75d0*R*dCOS(2.0*QZ))/ROOTRO
   DO 802 I=1,3,1
     D(I,I+3)=-C(1)*C(2)*C(3)
     D(I+3,I)=D(I,I+3)
 802 CONTINUE
   D(1,5)=S(1)*S(2)*C(3)+.00000011
   D(1,6)=S(1)*C(2)*S(3)+.00000021
   D(2,6)=C(1)*S(2)*S(3)+.00000011
   D(5,1)=D(1,5)+.00000011
   D(2,4)=D(1,5)+.00000011
   D(4,2)=D(1,5)+.00000021
   D(6,1)=D(1,6)+.00000011

  CALL PQR(D,6,W2,wmax)
```