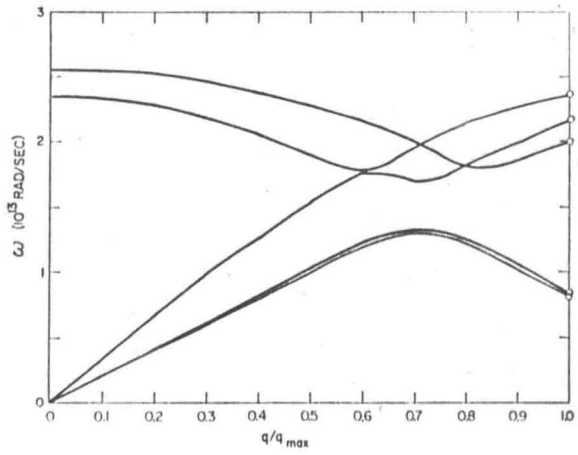

FIG. 5. Dispersion curves for white tin along [110] direction in the Brillouin zone using Mason and Bömmel elastic data.

This condition is well satisfied for the constants of Mason and Bömmel, but for Rayne and Chandrasekhar's data it is not.

The effect of the inconsistency is to lower the quasi-transverse branch by 40% and raise the quasilongitudinal branch by 10% along the [101] direction. All other branches along the principal directions including the pure transverse branch along the [101] direction are unaffected.

The resulting dispersion curves are shown in Figs. 1–3. For comparison Figs. 4–6 show the dispersion curves obtained in WLD. The value of the optical frequencies at $\mathbf{q}=\mathbf{0}$ are larger than in WLD. This is necessary in order to keep the optic-acoustic interaction small. In order to remove the condition on the elastic constants imposed by the A-S model one needs to consider a full tensor force model. This, however, will introduce more parameters which obviously could not be determined without experimental dispersion curves. In WLD it is shown that, for any atomic force model, it is necessary to include at least fourth neighbors in order to be consistent with elastic theory.

III. $2W$ FOR WHITE TIN

White tin has a body-centered tetragonal structure with two atoms per unit cell. The structure is two interpenetrating body centered tetragonal lattices with lattice basis (0,0,0), $(0,\frac{1}{2},\frac{1}{4})$. The superscript α is left out in what follows since the constant $2W$ must be the same for either lattice.

Equation (2) can be expressed as an inner product

$$2W=R(\rho,H\rho), \qquad \rho=(\rho_x,\rho_y,\rho_z), \tag{10}$$

where the elements of the H matrix are given by

$$H_{n,m}=\sum_q \sum_j g[\omega(q,j)]\mathbf{e}_n(q,j)\mathbf{e}_m{}^*(q,j). \tag{11}$$

TABLE I. Room temperature elastic constants for white tin (in units 10^{11} dyn cm^{-2}).

Constants	Mason and Bömmel	Rayne and Chandrasekhar
C_{11}	7.33	7.23
C_{33}	8.74	8.840
C_{44}	2.19	2.203
C_{66}	2.25	2.400
C_{12}	2.38	5.94
C_{13}	2.48	3.58

When the coordinate axes are chosen to lie along the principal axis of the crystal, $2W$ must be a quadratic function of the components of ϱ. Hence,

$$2W=R\{\rho_x{}^2H_{xx}+\rho_y{}^2H_{yy}+\rho_z{}^2H_{zz}\}, \tag{12}$$

or

$$=R\{(\rho_x{}^2+\rho_y{}^2)H_{xx}+\rho_z{}^2H_{zz}\}, \tag{13}$$

since the crystal has a fourfold axis of symmetry. It is convenient to express Eq. (13) in the form

$$2W=RH_{zz}(T)\{\epsilon(T)-\mu^2[\epsilon(T)-1]\},$$

where $\epsilon(T)=H_{xx}(T)/H_{zz}(T)$, $\mu=\cos\theta$, θ is the angle between ϱ and the principal axis.

IV. RESULTS

In order to calculate the constant $2W$ the vibration frequencies and polarization vectors for an arbitrary propagation vector $\mathbf{q}$ were determined using the axially symmetric lattice dynamics model described in a previous paper.[9]

The H_{xx} and H_{zz} matrix elements [Eq. (11)] were evaluated by integrating over $\frac{1}{16}$ of the Brillouin zone appropriate to white tin. This portion of the Brillouin zone was divided into two regions which were transformed into unit cubes by nonlinear transformations. A triple Gaussian quadrature was used to evaluate the resulting integrals.

The 6×6 dynamical matrix for white tin was diagonalized by a 2×2 Jacobi rotation procedure at 1024 points in each region. The polarization vectors for

TABLE II. A–S force constants (in units of 10^4 dyn cm^{-1}).

Constants	I[a]	II[b]
K_1 (1,12)	0.9183	0.2945
C_2 (1,12)	1.515	1.472
K_1 (2,11)	1.757	1.551
C_2 (2,11)	0.7575	−0.7362
K_1 (3,12)	1.276	2.446
C_2 (3,12)	−0.736	0.7404
K_1 (4,11)	0.4206	0.7054
C_2 (4,11)	−0.1979	−0.6688

[a] Using Mason and Bömmel elastic data.
[b] Using Rayne and Chandrasekhar elastic data.

[9] G. W. Lehman, T. Wolfram, and R. E. DeWames, Phys. Rev. 128, 1593 (1962).