tin in the center-of-mass system was discussed. The dynamic equations in this system are

$$\mathfrak{D}(q)\begin{pmatrix}\mathbf{x}_1\\ \\ \mathbf{x}_2\end{pmatrix}=\omega^2\begin{pmatrix}\mathbf{x}_1\\ \\ \mathbf{x}_2\end{pmatrix}, \tag{4}$$

where $\mathfrak{D}(q)$ is the dynamic supermatrix in the center-of-mass system with elements

$$\begin{aligned}\mathfrak{D}_{11}(\mathbf{q})&=D_{11}+\mathrm{Re}D_{12},\\ \mathfrak{D}_{12}(\mathbf{q})&=\mathfrak{D}_{21}(q)=-\mathrm{Im}D_{12},\\ \mathfrak{D}_{22}(\mathbf{q})&=D_{11}-\mathrm{Re}D_{12},\end{aligned} \tag{5}$$

and the D_{ij} are 3×3 supermatrices described in WLD. The vector $\mathbf{x}_1$ is the "pure" acoustical (in-phase) motion of the two sublattices and $\mathbf{x}_2$ is the "pure" optical (out-of-phase) motion. Using partitioning, we obtain the dynamic equations for the acoustic frequencies

$$\{(\mathfrak{D}_{11}-\omega^2)-\mathfrak{D}_{12}(\mathfrak{D}_{22}-\omega^2)^{-1}\mathfrak{D}_{12}\}x_1=0. \tag{6}$$

This equation is exact and shows that the acoustic frequencies are lowered by the presence of optical modes. The eigenvalues of $\mathfrak{D}_{11}$ and $\mathfrak{D}_{22}$ are the "pure" acoustical and optical frequencies, respectively. $\mathfrak{D}_{12}$ is the optic-acoustic interaction matrix. As $\mathbf{q}\rightarrow0$ the eigenvalues of $\mathfrak{D}_{11}$ and $\mathfrak{D}_{12}$ vanish. The matrix $\mathfrak{D}_{22}$, however, approaches a diagonal form with large constant eigenvalues, the optical frequencies. $(\mathfrak{D}_{22}-\omega^2)^{-1}$ can be expanded in a power series in $\mathfrak{D}_{22}^{-1}$,

$$(\mathfrak{D}_{22}-\omega^2)^{-1}=\mathfrak{D}_{22}^{-1}+\omega^2\mathfrak{D}_{22}^{-2}+\omega^4\mathfrak{D}_{22}^{-3}+\cdots. \tag{7}$$

This series converges very rapidly in the L-W limit since $[\omega\rightarrow0]$ while the eigenvalues of $\mathfrak{D}_{22}$ approach 10^{26} sec^{-2}. In the elastic limit one retains only terms of order q^2 so that the acoustic matrix reduces to

$$\{(\mathfrak{D}_{11}-\omega^2)-\mathfrak{D}_{12}\mathfrak{D}_{22}^{-1}\mathfrak{D}_{12}\}_{q\rightarrow0}. \tag{8}$$

The interaction matrix, $\mathfrak{D}_{12}$, is proportional to q^2 for crystals with an inversion center and consequently the second term in Eq. (8) is proportional to q^4 and may be neglected. On the other hand, for crystals without a center inversion, $\mathfrak{D}_{12}$ is proportional to $\mathbf{q}$ so that the optic-acoustic correction must be retained. Physically, however, we expect the correction to be small compared to "pure" acoustic frequencies. In WLD, the frequency spectrum for white tin was calculated using the elastic constants reported by Mason and Bömmel (see Table I). In this case the correction term could be ignored since it caused only negligible corrections (about 3%). The elastic constants reported by Rayne and Chandrasekhar,[7] (see Table I) also by House and Vernon,[8] imply in our model a much larger optic-acoustic interaction. In addition, these constants give rise to a much lower transverse acoustic branch along the [110] direction. Consequently, it is necessary to use Eq. (8) to determine the atomic force constants. Equating Eq. (8) to the elastic matrix as discussed in WLD yields quadratic algebraic equations relating the atomic force constants to the elastic constants. The value of ω_{av} and t were chosen according to the procedure in WLD. The A-S atomic force constants for the two calculations are given in Table II.

Using the elastic data of Mason and Bömmel it was possible to satisfy all equations within the experimental error in the elastic constants. However, with the elastic data of Rayne and Chandrasekhar, it was not possible to obtain total consistency among all the equations. This resulted because the A-S model implies that

$$C_{44}-C_{13}-C_{66}+C_{12}=0. \tag{9}$$

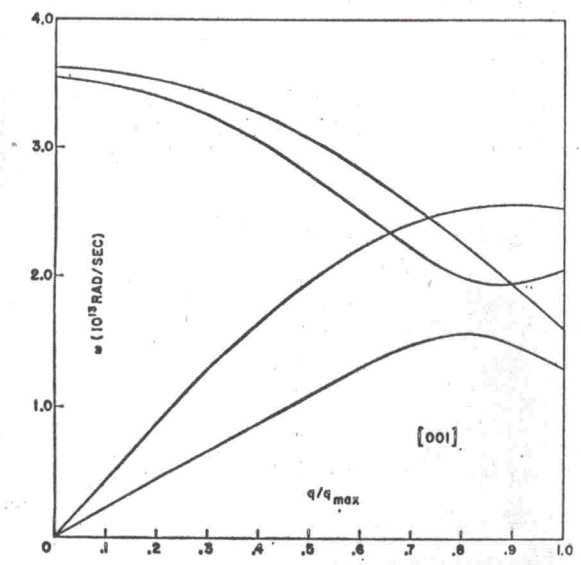

FIG. 3. Dispersion curves for white tin along [001] direction in the Brillouin zone using Rayne and Chandrasekhar elastic data.

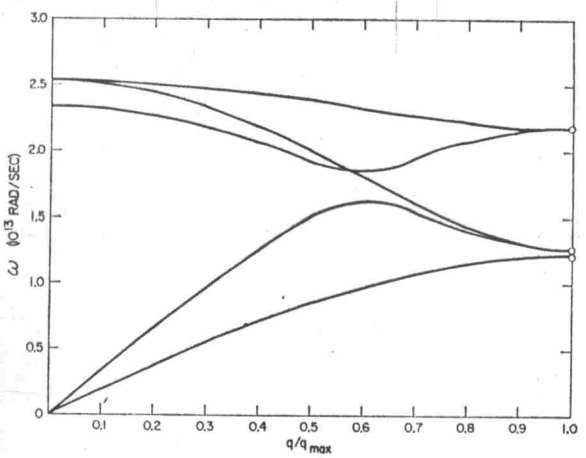

FIG. 4. Dispersion curves for white tin along [100] direction in the Brillouin zone using Mason and Bömmel elastic data.

[8] D. G. House and E. V. Vernon, Brit. J. Appl. Phys. 11, 254 (1960).