

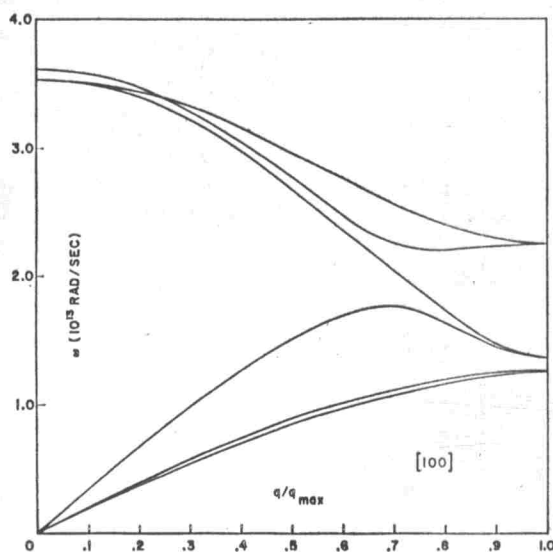


FIG. 1. Dispersion curves for white tin along [100] direction in the Brillouin zone using Rayne and Chandrasekhar elastic data.

$$g[\omega(q, j)] = \frac{1}{N\hbar\omega(q, j)} \left\{ \frac{1}{\exp[\hbar\omega(q, j)/kT] - 1} + 1 \right\}, \quad (3)$$

where N is the number of unit cells, R is the recoil energy of a free emitting atom, $\hbar$ is Planck's constant divided by 2π , k is the Boltzmann constant, T is the absolute temperature, $\mathbf{q}$ is the propagation vector, and j is the polarization of a vibrational wave of the crystal. α refers to the specific lattice from which the γ ray is being emitted or absorbed, $\mathbf{e}^\alpha$ is a unit vector in the direction of emission of the γ ray, $\mathbf{e}^\alpha(q, j)$ is the polarization vector of the vibrational wave.

The purpose of this paper is to provide accurate theoretical values for the Debye-Waller factor for white tin in the temperature region of the harmonic approximation. Calculations of this type are necessary in order to determine the extent to which the existing theory agrees with experimental results.⁴ In this paper, Eq. (2) is evaluated using the theoretical frequency spectrum and polarization vectors for white tin calculated from the elastic data.

In a previous paper,⁵ referred to as WLD, the fre-

⁴ A rough order of magnitude calculation of the anisotropy ratio for tin in agreement with our results has been reported recently by Yu. Kagan. [Dokl. Akad. Nauk SSSR 140, 794 (1961) [translation: Soviet Phys.—Doklady 6, 881 (1962)]]. However, in view of the methods used by Kagan in evaluating this ratio, we conclude that this agreement is accidental, inasmuch as the optical modes were not included. Kagan's expressions require a detailed knowledge of the density of states—a quantity not to be obtained in any simple manner analytically for a real crystal. His density of states is derived from a simplified nearest neighbor lattice dynamics model in which the dynamical matrix is diagonal and consequently inconsistent with the elastic-dynamic matrix. In addition, the model does not apply to the actual structure of tin. Having omitted the optical mode contributions, the expressions derived are not valid since the optical modes contribute significantly, particularly at low temperatures as is shown from specific heat data and by our detailed calculations.

⁵ T. Wolfram, G. W. Lehman, and R. E. DeWames, Phys. Rev. 129, 2483 (1963).

quency spectrum for white tin was calculated using the elastic constants reported by Mason and Bömmel.⁶

In this paper we also calculate the frequency spectrum using the elastic constants of Rayne and Chandrasekhar.⁷ In Sec. II the dynamic matrix for the acoustic frequencies is obtained including the interaction of the optical motion. In the long-wavelength limit this matrix reduces to an effective elastic matrix in which the effect of the relative motion of the two sublattices is retained. The method of calculation with the resulting dispersion curves is also presented.

In Sec. III, the constant $2W$ is expressed as a quadratic function of the components of $\mathbf{e}^\alpha$. The method and results of our calculations are presented in Sec. IV.

II. EFFECT OF OPTICAL MOTION ON THE ACOUSTIC MATRIX

In this section we consider the interaction of the optical and acoustical modes and show that the acoustic frequencies are in general depressed. This depression can be understood in terms of a mixing of relative sublattice motion into the "pure" acoustic motion in which the two sublattices are moving as a unit. In the long-wavelength (L-W) limit the optic-acoustic interaction is proportional to q^4 for crystals with an inversion center but proportional to q^2 otherwise. Consequently, the elastic properties of crystals without an inversion center, such as white tin, will contain an optic-acoustic interaction term while crystals with an inversion center will not. In this section we obtain the corrected L-W acoustic matrix.

In WLD, the form of the dynamic matrix for white

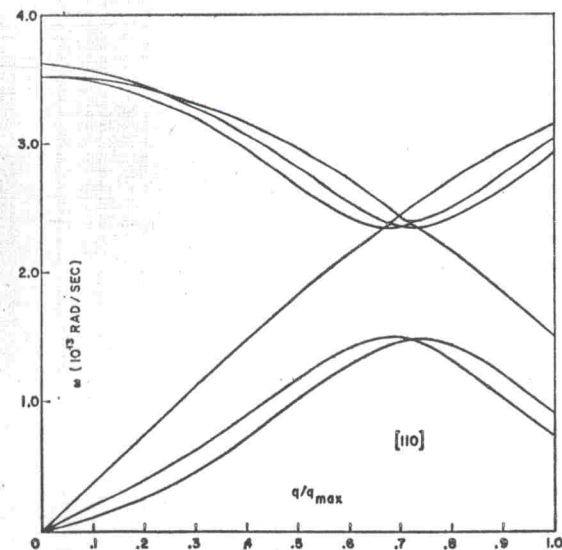


FIG. 2. Dispersion curves for white tin along [110] direction in the Brillouin zone using Rayne and Chandrasekhar elastic data.

⁶ W. P. Mason and H. E. Bömmel, J. Acoust. Soc. Am. 28, 930 (1956).

⁷ J. A. Rayne and B. S. Chandrasekhar, Phys. Rev. 120, 1658 (1960).