

TABLE III. Comparison of experimental and calculated values for the polycrystal Debye-Waller factor.

$T(^{\circ}\text{K})$	Wiedemann <sup>a</sup> <i>et al.</i>	Boyle <i>et al.</i>	Barloutand <sup>b</sup> <i>et al.</i>	Alekseyevsky <i>et al.</i>	I <sup>c</sup>	II <sup>d</sup>	Debye model $\theta_D=142^{\circ}\text{K}$
4	(0.53), (0.60)				0.63	0.61	0.73
20	(0.52), (0.59)				0.61		0.70
77	(0.39), (0.40)	(0.40)		(0.32 ± 0.06)	0.40	0.37	0.46
90			(0.30 ± 0.07), (0.32 ± 0.015)				
150		0.22			0.22	0.18	
300		0.035		(0.061 ± 0.015)	0.053	0.036	0.07
400		0.009				0.011	
500		0.002			0.008	0.004	0.012

<sup>a</sup> W. H. Wiedemann, P. Kienle, and F. Pobell, Z. Physik 166, 109 (1962).  
<sup>b</sup> R. Barloutand, J. O. Picon, and C. Tzara, Compt. Rend. 250, 2705 (1960).  
<sup>c</sup> Using Mason and Bömmel elastic data.  
<sup>d</sup> Using Rayne and Chandrasekhar elastic data.

points lying outside the fundamental  $\frac{1}{16}$  of the Brillouin zone were obtained by means of symmetry operations of the  $D_{4h}$  group. Several checks were made to insure that our values of  $H_{m,m}$  were independent of order of the Gaussian quadrature.

The experimental and calculated temperature dependence of the polycrystalline Debye-Waller factor is given in table III showing good agreement from 0 to 300°K. The values calculated using Rayne and Chandrasekhar's elastic data seem to give the best over-all fit; however, with the present experimental accuracy it does not seem possible to select between the two calculations. For comparison, the temperature dependence of Debye-Waller factor calculated from the Debye approximation with  $\theta_D=142^{\circ}\text{K}$ , as suggested in a previous analysis<sup>10</sup> is also shown in Table III. Clearly, our results indicate that the Debye model does not give a good representation of the frequency spectrum of tin and that one is not justified in accounting for the difference between experimental values and calculated values using the Debye approximation by introducing higher order corrections such as anharmonicities. The deviation of experimental values from calculated values using A-S model above 300°K can now probably be attributed to higher order corrections. The effect of anharmonicities is presently being investigated.

 TABLE IV. Temperature dependence of  $H_{zz}(T)$  and  $\epsilon(T)$ .

$T(^{\circ}\text{K})$	$H_{zz}(T)^a$ (in units of $10^3 \text{ eV}^{-1}$ )	$\epsilon(T)^a$	$H_{zz}(T)^b$ (in units of $10^3 \text{ eV}^{-1}$ )	$\epsilon(T)^b$
4	0.169	1.106	0.174	1.106
6	0.170	1.106	0.175	1.106
15	0.175	1.109	0.183	1.109
50	0.233	1.15	0.260	1.14
77	0.304	1.17	0.345	1.15
150	0.526	1.19	0.606	1.16
300	1.01	1.2	1.17	1.17
400	1.34	1.2	1.56	1.17
500	1.68	1.2	1.95	1.17

<sup>a</sup> Using Mason and Bömmel elastic data.  
<sup>b</sup> Using Rayne and Chandrasekhar elastic data.

<sup>10</sup> A. J. F. Boyle, D. St. P. Bunbury, C. Edwards, and H. E. Hall, Proc. Phys. Soc. (London) A77, 129 (1961).

The temperature dependence of the function  $H_{zz}(T)$  and the anisotropy ratio  $\epsilon(T)$  is given in Table IV. The anisotropy ratio is found to be only slightly temperature sensitive in agreement with Kagan's results.<sup>4</sup>

We are currently aware of two recent attempts at measuring the anisotropy ratio of  $f_x/f_z = e^{-RH_{zz}}/e^{-RH_{zz}}$ . One of these measurements has been attempted by Alekseyevsky *et al.*<sup>11</sup> and their conclusion is that  $f_x/f_z=1.4$  over the whole temperature range. Their calculated  $f_x/f_z$  was determined from experimental data corrected for quadrupole effects.

It is apparent that the conclusions of Alekseyevsky *et al.* are in disagreement with our theoretical prediction. In fact, their conclusions that  $f_x/f_z=1.4$  over the 80–300°K range imply that the anisotropy ratio  $\epsilon(T)$ , is not only strongly temperature dependent but increases as the temperature increases, which implies that the lattice anisotropy is decreasing as the temperature increases. This is difficult to believe because if the mean square displacement along the [001] is larger at low

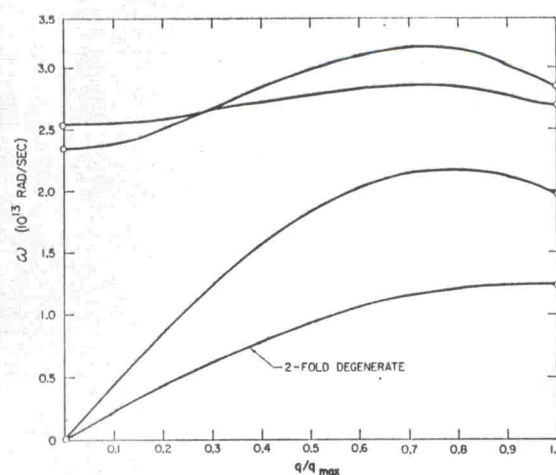


FIG. 6. Dispersion curves for white tin along [001] direction in the Brillouin zone using Mason and Bömmel elastic data.

<sup>11</sup> N. E. Alekseyevsky, Pham Zuy Hien, V. G. Shapiro, V. S. Shunel, Zh. Eksperim. i Teor. Fiz. 43, 790 (1962) [translation: Soviet Phys.—JETP 16, 559 (1963)].