

temperatures than that along the [100] direction in the harmonic region one would expect their ratio to be an increasing function of temperature (since the functional dependence on frequency goes from $\langle 1/\omega \rangle$ to $\langle 1/\omega^2 \rangle$ at high temperatures). Furthermore, the thermal expansion data show that the thermal expansion coefficient along the [001] is higher than along the [100]; this should still further increase the difference.

The other measurement is that of Meechan *et al.*¹² of our laboratory who have obtained essentially the same value for f_x/f_a at room temperature but no measurable difference for f_x/f_a at 100°K.

This experimental discrepancy must be resolved be-

TABLE V. Comparison of experimental and calculated values of the Debye-Waller factor along three crystal axes.

T(°K)	Aleksyevsky <i>et al.</i>		A-S model			
	77	293	I ^a		II ^b	
			77	293	77	293
[001]	0.24±0.05	0.054±0.01	0.46	0.074	0.41	0.05
[101]		0.072±0.01		0.05		0.033
[100]	0.36±0.06	0.076±0.01	0.39	0.045	0.36	0.03

^a Using Mason and Bömmel elastic data.

^b Using Rayne and Chandrasekhar elastic data.

fore we can make meaningful comparison between theory and experiment.

The experimental and calculated angular dependence of the Mössbauer intensity for several temperatures is shown in Table V. The anisotropy ratios are compared in Table VI. Table VII gives the calculated and experimental specific¹³ heat from 1 to 300°K. As expected, the calculated specific heat values using Rayne and Chandrasekhar's elastic data is slightly higher than that calculated using Mason and Bömmel's elastic data.

¹² C. J. Meechan, A. H. Muir, U. Gonser, H. Wiedersich, *Bull. Am. Phys. Soc.* **7**, 600 (1962).

¹³ C. A. Shiffman, The Heat Capacities of the Elements below Room Temperature, General Electric Research Laboratory (unpublished).

TABLE VI. Comparison of experimental and calculated values of the anisotropy ratio $\epsilon(T)$.

T(°K)	Aleksyevsky <i>et al.</i>	$\epsilon(T)$	
		I ^a	II ^b
77	0.715	1.17	1.15
300	0.883	1.2	1.17

^a Using Mason and Bömmel elastic data.

^b Using Rayne and Chandrasekhar elastic data.

Between 6-15°K the calculated values are low. It was impossible to raise the lattice contribution to the specific heat in that temperature range without changing the low temperature agreement of C_v and the Debye-Waller factor.

TABLE VII. Comparison of experimental and calculated values for the total specific heat of white tin^a (in units of cal mole⁻¹ deg⁻¹).

T(°K)	C_v (exp)	C_v (I) ^b	C_v (II) ^c
1	0.00046	0.00042	0.00045
2	0.0014	0.0011	0.0015
3	0.0032	0.0027	0.0042
4	0.0067	0.0053	0.0074
6	0.036	0.015	0.021
15	0.64	0.25	0.29
50	3.68	3.10	3.08
150	5.85	5.55	5.53
300	6.3	5.97	5.97

^a $\gamma = 3.5 \times 10^{-4}$ cal mole⁻¹ deg⁻¹.

^b Using Mason and Bömmel elastic data.

^c Using Rayne and Chandrasekhar elastic data.

ACKNOWLEDGMENTS

The authors are particularly indebted to C. J. Meechan and A. H. Muir for numerous discussions concerning the experimental work on Sn. We also wish to acknowledge discussions with M. H. Cohen, U. Gonser, V. Heine, and H. Wiedersich on the subject matter of this paper.