

TABLE III. $C(T)$ for copper (in units of 10^2 eV^{-1}).

$T(^{\circ}\text{K})$	Flinn <i>et al.</i> Experimental values		C.F. model	Jacobsen	White	A-S	Debye model $\theta_D=335^{\circ}\text{K}$
	θ_D	$C(T)$					
4	320 ± 10	0.544 ± 0.02	0.552	0.579	0.537	0.570	0.520
20	320 ± 10	0.588 ± 0.02	0.566	0.593	0.548	0.582	0.532
80	320 ± 10	0.755 ± 0.04	0.762	0.808	0.733	0.779	0.697
300	315 ± 10	2.17 ± 0.14	2.10	2.29	2.03	2.18	1.93
400	300 ± 10	3.14 ± 0.25	2.77	3.02	2.67	2.87	2.50

for aluminum determined by Walker from his experimental dispersion curves. The experimental and calculated temperature dependence of $C(T)$ for copper is given in Table III. For comparison we calculated $C(T)$

using a Debye model, the results of these calculations are also shown in this table.

From the results in Table III we conclude that the experimental determination of the Debye-Waller factor for pure host lattices of cubic symmetry is not sensitive enough to distinguish between the various models. Models inconsistent with experimental dispersion curves such as the C.F. model and White's full tensor model give essentially the same Debye-Waller factor.

The results of the calculations for aluminum using Walker's force constants are given in Table IV. Using the A-S force constants the values of $C(T)$ are higher than Walker's by 1% at 0°K and by 4% at 400°K . Only a small difference is expected since Walker's constants are essentially axially symmetric.

TABLE IV. $C(T)$ for aluminum (in units of 10^2 eV^{-1}).

$T(^{\circ}\text{K})$	Walker	Debye model ($\theta_D=382^{\circ}\text{K}$)
4	0.471	0.459
20	0.478	0.464
80	0.598	0.583
300	1.54	1.50
400	2.02	1.96

Temperature Dependence and Anisotropy in the Debye-Waller Factor for White Tin

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The Debye-Waller factor, e^{-2W} , for tin is calculated using the A-S (axially symmetric) lattice dynamics model described in an earlier paper. The Debye continuum approximation is found to be unsatisfactory because the optical modes contribute significantly even at low temperatures. Calculated and experimental values determined from Mössbauer measurements are in excellent agreement in the temperature range from 0 to 300°K . Discrepancies above 300°K are attributed to higher order corrections such as anharmonicity and diffusion effects. In tin, the Debye-Waller factor depends upon the direction of gamma ray emission with the ratio $2W_z/2W_x$ varying from 1.1 to 1.2 for $T=0^{\circ}\text{K}$ and $T=300^{\circ}\text{K}$, respectively. The calculated anisotropy in $2W$ is compared with available experimental data. Dispersion curves and values of $2W$ calculated using Rayne and Chandrasekhar elastic data are compared with those calculated using Mason and Bömmel elastic data. The effect of the relative motion of the two sublattices on the elastic properties of tin is discussed and found to be important for the elastic constants of Rayne and Chandrasekhar.

I. INTRODUCTION

THE probability of a gamma-ray emission without energy transfer to or from the lattice^{1,2} and the temperature dependence of the atomic structure factor in the reflection of x rays³ is given by

$$f = e^{-2W} \quad (1)$$

where $2W$ is related to the mean square displacement of an atom along a definite direction.

Since the experimental determination of f for tin has only been investigated through a study of the temperature dependence of recoil-less γ emission the constant $2W$ is defined for this specific case. Hence,

$$2W = R \sum_q \sum_j [\rho^{\alpha} \cdot \mathbf{e}^{\alpha}(q, j)]^2 g[\omega(q, j)], \quad (2)$$

¹ R. L. Mössbauer, *Z. Physik* **151**, 124 (1958).

² W. E. Lamb, Jr., *Phys. Rev.* **55**, 190 (1939).

³ R. W. James, *The Optical Principles of the Diffraction of X-Rays* (G. Bell and Sons, London, 1953).