Reprinted from THE PHYSICAL REVIEW, Vol. 131, No. 2, 529–534, 15 July 1963
Printed in U. S. A.

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

R. E. DEWAMES, T. WOLFRAM, AND G. W. LEHMAN
North American Aviation Science Center, Canoga Park, California
(Received 11 March 1963)

The Debye-Walker 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 anharmonicities and diffusion effects. In tin, the Debye-Waller factor depends upon the direction of gamma ray emission with the ratio $2W_x/2W_z$ varying from 1.1 to 1.2 for $T=0°K$ and $T=300°K$, 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 rays[3] is given by

$$f=e^{-2W} \tag{1}$$

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,

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

[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).