

III. SOLID STATE PHYSICS

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A. FREQUENCY SPECTRUM OF MAGNESIUM

Application of the Born-von Kármán theory of lattice dynamics to a central-force model of the hexagonal close-packed metals was recently reported (1). The frequency-distribution spectrum of normal modes for this model has been approximated by a root-sampling technique in which force constants calculated from the elastic constants of magnesium (2) at 0° K were used. The frequency spectrum, $g(\nu)$, is so defined that $g(\nu)d\nu$ is the number of normal modes in the interval from ν to $\nu + d\nu$. The spectrum may be approximated numerically by solving the lattice dynamical secular equation at a number of points in reciprocal space and determining the number of roots (properly weighted according to the degeneracy of the point in reciprocal space) that lie within given frequency intervals. This process was carried out on the Whirlwind I computer for a mesh of 429 points which lie in that twenty-fourth part of the Brillouin zone which is irreducible under symmetry. The basic frequency interval chosen was $0.125 \times 10^{12} \text{ sec}^{-1}$; at low frequency larger intervals were used, and a smooth curve drawn. The normalized frequency spectrum of this model of magnesium is given in Fig. III-1, in which both the histogram and the smooth curve up to $3.75 \times 10^{12} \text{ sec}^{-1}$ are shown.

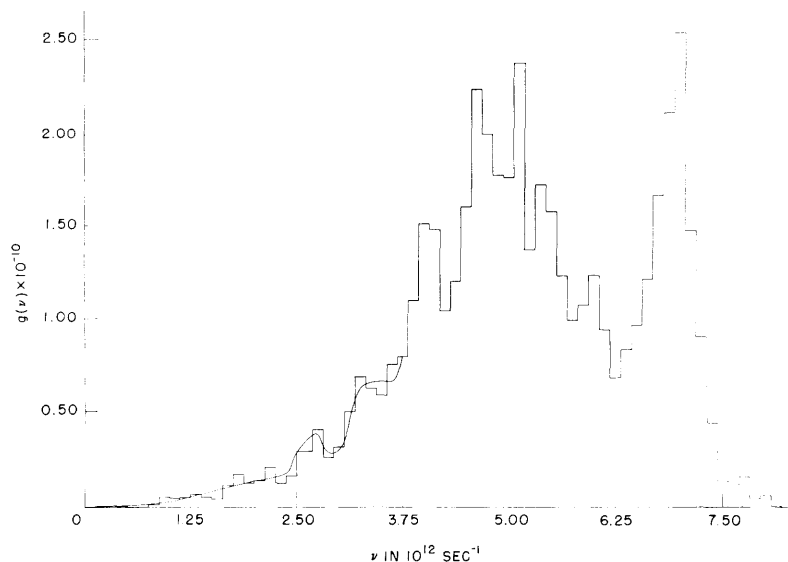


Fig. III-1. Frequency-distribution spectrum, $g(\nu)$, for a central-force model of magnesium at 0° K.

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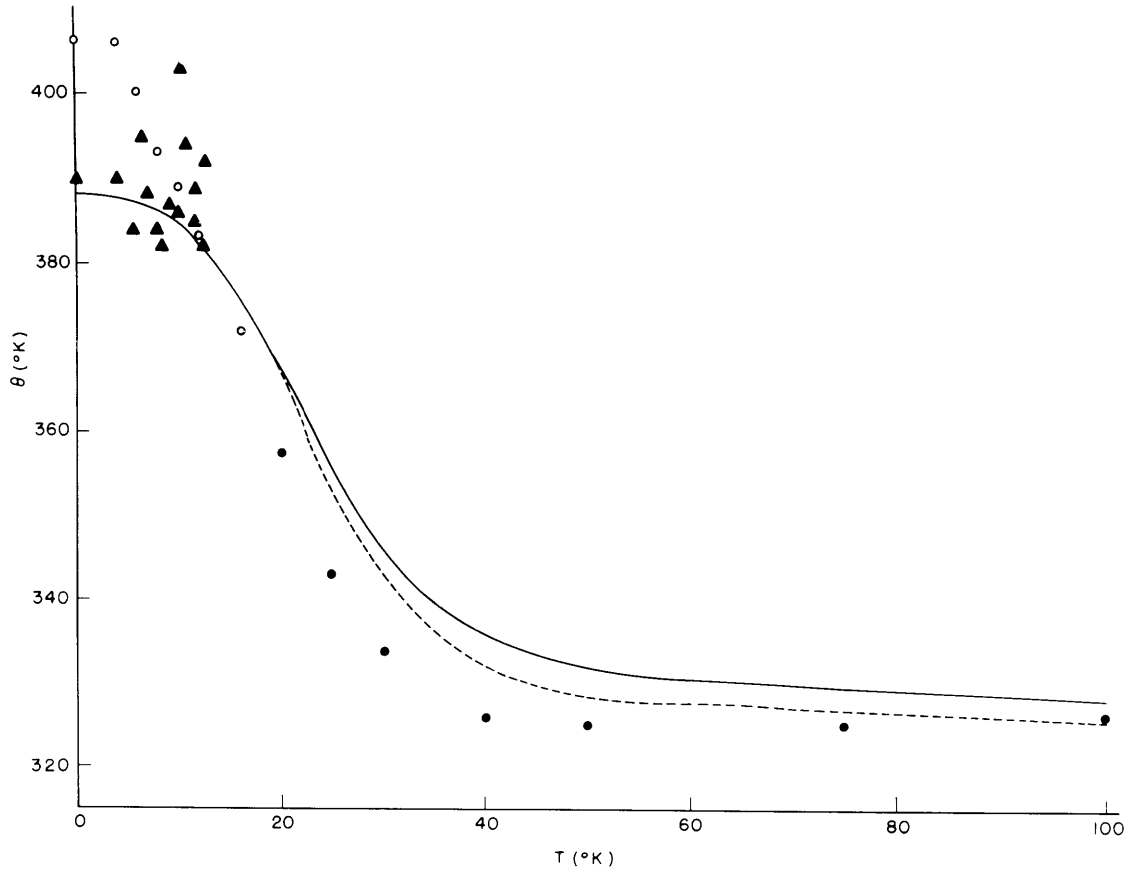


Fig. III-2. Equivalent Debye θ versus temperature for magnesium.
 ○ experimental values of Smith
 ● calculated from the data of Craig et al.
 △ obtained from the data of Logan et al.
 — theoretical result obtained from the frequency spectrum shown in Fig. III-1.
 -- based on 217 points in reciprocal space.

The lattice heat capacity at constant volume is given by the expression

$$C_V = k \int_0^{\nu_L} g(\nu) (h\nu/kT)^2 e^{h\nu/kT} d\nu / (e^{h\nu/kT} - 1)^2 \quad (1)$$

where ν_L is the maximum vibrational frequency, $8.098 \times 10^{12} \text{ sec}^{-1}$ for magnesium. The lattice heat capacity was obtained by a numerical integration of Eq. 1 in which the frequency spectrum given in Fig. III-1 was used. A comparison of the calculated C_V with experimental data in the range from 0° K to 100° K is presented in Fig. III-2. This comparison was made, as is customary, in terms of an equivalent Debye temperature, θ . The experimental points are those of Logan, Clement, and Jeffers (3);

Smith (4); and Craig, Krier, Coffey, Bates, and Wallace (5).

The dotted curve given in Fig. III-2 represents values of θ calculated as described above from a spectrum derived from solutions of the secular equation at only 217 points in reciprocal space. The spectrum agreed in all major features with the spectrum shown in Fig. III-1, and the θ -values calculated from it are seen to be in fairly close agreement with those calculated from the spectrum based on 429 points. We are therefore inclined to attribute the disagreement between the calculated curve and the experimental points to the inadequacies of the model or inaccuracies in the parameters rather than to a root sampling that is not sufficient to characterize the spectrum. It may be said, however, that the agreement obtained for magnesium is as good or better than that which has been recently obtained for other metals.

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References

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