where the sum is over all calculated frequencies, and

$$E(x) = \frac{x^2 e^x}{(e^x - 1)^2}$$

is the reduced Einstein specific heat for a single oscillator of frequency, ω. The weight function $w(q)$ is the number of wave vectors in the entire Brillouin zone equivalent to q, where q is one of the 47 points in $\frac{1}{48}$ of the Brillouin zone.

boundary. These low frequencies are responsible for the sharp minimum in the Debye curve near 20°K. The point ion models predicted considerably higher frequencies and did not reproduce the minimum. Low frequency transverse acoustic modes have been found from inelastic neutron scattering measurements in other semiconductors.[18,27,28]

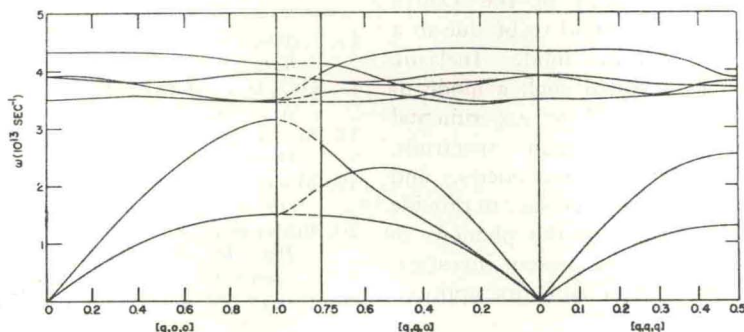The optic modes were found to be quite flat, and since these frequencies were fitted at $q = 0$,

FIG. 7. Phonon dispersion curves for Mg₂Sn calculated from a shell model. The low frequency transverse acoustic modes are responsible for the sharp minimum in the Debye temperature near 20°K.

It is customary to display results of specific heat calculations or measurements in terms of the Debye curve as a function of temperature. In Fig. 5, we have shown the results of our calculations for the shell model and the two point ion models along with the experimental results of JELINEK et al.[4] It can be seen that the shell model calculations agreed with experiment better than either point ion model calculations especially at the low temperature minimum in the Debye curve. None of the models agreed particularly well with the experimental curve above 140°K, where the Debye temperature decreases steadily. A similar high temperature decrease can be seen in some alkali halides[22] and III–IV compounds.[15] Generally, such a decrease in θ_D has been attributed to anharmonic effects, which are not included in a harmonic approximation to lattice dynamics.

The lattice vibration frequencies calculated for the shell model are shown in Fig. 7 for wave vectors, q, along the principal symmetry directions. Our results showed that the transverse acoustic modes have very low frequencies, even at the zone

the calculated curves should be reasonably accurate. The Raman modes, however, were not fitted at $q = 0$ since ω_R was not known; the Raman frequency was sensitive to the Mg–Mg force constant α_3. We picked α_3 so that the Debye curve agreed with experiment. Decreasing α_3, for example, caused a vertical shift downward of the Debye curve below the experimental value and an over-all lowering of the Raman mode frequencies.

SUMMARY

The elastic properties of Mg₂Sn and the related compounds Mg₂Si and Mg₂Ge are quite similar to those of a number of common semiconductors. An interesting feature of the Mg₂X compounds, however, is the small departure from the condition of elastic isotropy, especially in Mg₂Si and Mg₂Ge.

The SZIGETI[25,26] charge, which was the effective ionic charge of the Mg ions in our shell model, was found to be approximately 0·3e for Mg₂Sn. (It was also found to be about 0·3e in

Mg_2Si and Mg_2Ge.) Such a small charge is consistent with the covalent nature of the bonding in these compounds, yet it is large enough to account for the infrared reflectivity spectrum which is characteristic of an ionic compound.

Calculations of the lattice vibration frequencies in Mg_2Sn could be compared with experiment only by comparing the calculated and experimental Debye curves. Good agreement was attained when the polarizability of the Sn was taken into account. The sharp minimum in the Debye temperature near $20°K$ was found to be due to a low-lying transverse acoustic mode. Inelastic neutron scattering has revealed such a mode in $Ge^{[18,27]}$ and $GaAs.^{[18,28]}$ More experimental information, such as the Raman spectrum, multiple phonon absorption frequencies, and inelastic neutron scattering, is necessary to provide a more accurate description of the phonons in Mg_2Sn, but, the results of the present investigation are thought to give a reasonable first approximation.

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APPENDIX

Following GANESAN and SRINIVASAN[24] we define the matrix of force constants between one ion and another. The matrix can be written most generally as

$$D = \begin{pmatrix} \phi_{xx} & \phi_{xy} & \phi_{xz} \\ \phi_{yx} & \phi_{yy} & \phi_{yz} \\ \phi_{zx} & \phi_{zy} & \phi_{zz} \end{pmatrix}$$

where, for example, $\phi_{zy} = (\partial^2\phi/\partial x\partial y)$ is evaluated at the equilibrium separation. ϕ is the two-body potential associated with the short range forces between one ion and another.

We list the matrix of force constants for the Sn core–Sn shell, nearest neighbor Mg–Sn, next nearest