The isotropy coefficient, $S = (C_{11} - C_{12})/2C_{44}$, which has the value 1 for an isotropic crystal, was found to be 0·84 for Mg$_2$Sn. The temperature dependence of the elastic constants is shown in Fig. 4. Sample lengths and densities were corrected for thermal expansion using the coefficient of linear expansion which was determined by
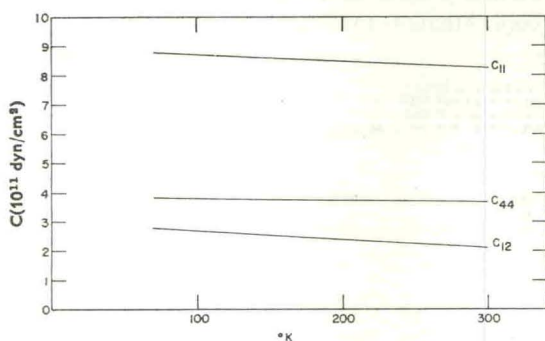


FIG. 4. Elastic constants of Mg$_2$Sn.

SHANKS.[13] He obtained a value of $0·99 \times 10^{-5}/°$K from the temperature dependence of the lattice constant as measured from X-ray diffraction patterns.

Listed in Table 1 are the elastic constants for a number of common semiconductors. It should be noted that Mg$_2$Sn is somewhat different from the related compounds Mg$_2$Si and Mg$_2$Ge. The elastic constants, especially $C_{11}$, are smaller, and Mg$_2$Sn is less isotropic than either Mg$_2$Si or Mg$_2$Ge. A similar reduction in the values of the elastic constants can be seen in a comparison of GaAs and GaSb and of InAs and InSb. In fact, the elastic constants of Mg$_2$Sn resemble those of GaSb except that $C_{12}$ is only about one-half of $C_{44}$ in Mg$_2$Sn. The relative magnitudes of the elastic constants, $C_{11} > C_{44} > C_{12}$, are the same as in Si and Ge. The Mg$_2$X compounds are more isotropic than any of the other semiconductors listed.

## INTERATOMIC FORCE MODELS

KAHAN et al.[3] have measured the high and low frequency dielectric constants, $\epsilon_\infty$ and $\epsilon_0$, and the reststrahl (transverse optic) frequency $\omega_{IT}$ for Mg$_2$Sn. They found $\epsilon_\infty = 15·5$, $\epsilon_0 = 23·75$, and $\omega_{IT} = 3·50 \times 10^{13}$ sec$^{-1}$. From the LYDDANE-

Table 1. *Elastic constants of some common semi-conductors*

| | $C_{11}$ (10 in. dyn/cm²) | $C_{12}$ | $C_{44}$ | $S = \dfrac{C_{11} - C_{12}}{2C_{44}}$ |
|---|---|---|---|---|
| Mg$_2$Si* | 12·1 | 2·2 | 4·64 | 1·07 |
| Mg$_2$Ge† | 11·79 | 2·30 | 4·65 | 1·02 |
| Mg$_2$Sn‡ | 8·24 | 2·08 | 3·66 | 0·84 |
| Si§ | 16·57 | 6·39 | 7·95 | 0·64 |
| Ge§ | 12·88 | 4·83 | 6·71 | 0·60 |
| GaAs‖ | 11·92 | 5·97 | 5·38 | 0·55 |
| GaSb‖ | 8·85 | 4·04 | 4·33 | 0·56 |
| InAs‖ | 8·33 | 4·53 | 3·96 | 0·48 |
| InSb‖ | 6·75 | 3·47 | 3·16 | 0·52 |

\* Ref. 1.
† Ref. 2.
‡ Present investigation.
§ Ref. 14.
‖ Ref. 15.

SACHS–TELLER[16] relation,

$$\frac{\omega_{IL}}{\omega_{IT}} = \sqrt{\left(\frac{\epsilon_0}{\epsilon_\infty}\right)},$$

we found the longitudinal optic frequency, $\omega_{IL}$, to have the value $4·33 \times 10^3$ sec$^{-1}$.

From our measurements of the elastic constants and the above optical constants, it appeared feasible to make a calculation of the phonon dispersion curves for Mg$_2$Sn. Three different force constant models were employed in our calculation. The first two, model I and model II, were point ion models, previously proposed by WHITTEN et al.[1] and CHUNG et al.[2] for Mg$_2$Si and Mg$_2$Ge. Models I and II differed only in the assumptions made concerning the short range forces between next nearest neighbors. The third model was a slight modification of the shell model as first proposed by DICK and OVERHAUSER[17] and successfully used by many authors.[18] Although few tests of the validity of our calculated phonon dispersion curves are currently available, it is clear that the shell model provided the best fit to the Debye curve as a function of temperature (see Fig. 5).

To construct a physically plausible picture of Mg$_2$Sn, apparently one must account for both an ionic character and a covalent character. The infrared reflectivity spectrum of Mg$_2$Sn is characteristic of an ionic compound. The difference in

the high and low frequency dielectric constants is also characteristic of an ionic compound.

The relative sizes of the elastic constants $C_{44}$ and $C_{12}$, however, resemble those of covalent semiconductors. In fact, MOOSER and PEARSON[19] have suggested that covalent bonding is necessary for $Mg_2Sn$ to be a semiconductor. In addition, the small energy gap, $0.33$ eV,[20] would indicate that $Mg_2Sn$ is not strongly ionic. Experimentally,

model was the polarizable Sn ion (that is, a shell isotropically and harmonically bound to an Sn ion core). The polarizability of the lighter Mg ions was neglected.

We modified the usual shell model[17,18] slightly in that we did not include a force between the positive ion (Mg) and the Sn shell, but we did include a force between the Mg ion and the Sn core. Attempts to include a Mg ion–Sn shell force,
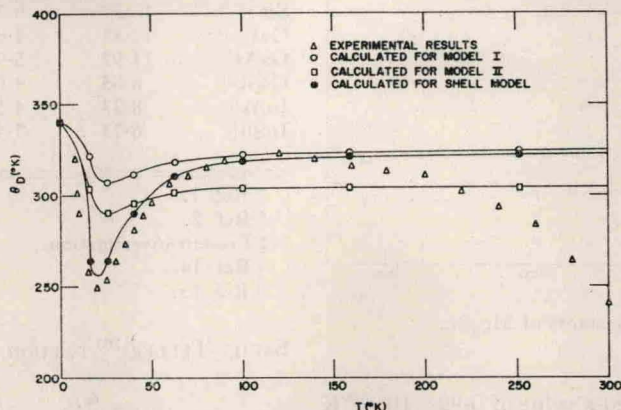


FIG. 5. The Debye temperature of $Mg_2Sn$ is shown as a function of temperature. Models I and II are point ion models. Best agreement with the experimental curve was obtained for the shell model which reproduced quite accurately the sharp minimum near $20°K$. The decrease in the experimental curve above $140°K$ is probably due to anharmonic effects.

LICHTER[21] has concluded that the bonding in $Mg_2Sn$ is predominantly covalent from an investigation of the growth of $Mg_2Sn$ crystals from non-stoichometric melts. Therefore, we have taken $Mg_2Sn$ to be partially ionic and partially covalent.

The three force constant models we have used all contained long range Coulomb forces arising from the ionic charges and short range forces between nearest neighbors resulting from the covalent bonds. The short range forces of model I can be described by nearest neighbor Mg–Sn forces, both central and non-central, and second nearest neighbor Mg–Mg and Sn–Sn forces, only central. Model II had central and non-central Mg–Sn forces, central and non-central Sn–Sn forces, and no Mg–Mg force at all. The shell model had central and non-central forces between Mg–Sn ions and Sn–Sn ions, with a small central Mg–Mg force. The salient feature of the shell

corresponding to the deformation dipole moment of KARO and HARDY,[22] gave poor agreement with the specific heat data. There may be some theoretical justification for neglecting the deformation dipole moment in $Mg_2Sn$. In an alkali halide, it is clear that the electronic distributions about the positive and negative ions repel one another when the ions are displaced from equilibrium and brought closer together. The repulsion of the electronic charge clouds gives rise to a deformation dipole moment. But when a substantial amount of covalent bonding is present (as in $Mg_2Sn$), it is not clear what the electronic distributions do, and it may be that the deformation dipole moments are small.

## DYNAMICS OF THE SHELL MODEL

We shall discuss only the dynamics of the shell model. The dynamics of the point ion models