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,

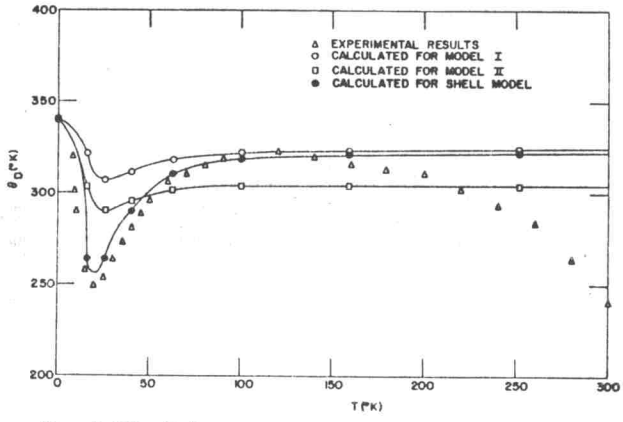

FIG. 5. The Debye temperature of Mg_2Sn is shown as a function of temperature. Models I and II are point ion models. Best agreement with the experimental curve was obtained for the shell model which reproduced quite accurately the sharp minimum near 20°K. The decrease in the experimental curve above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