

which are quite similar to the shell model have been discussed in detail.^(1,2)

The crystal structure of Mg₂Sn is the same as CaF₂. (See Fig. 6.) The lattice is face-centered cubic and the basis consists of a Sn ion at the origin and Mg ions at (a/4, a/4, a/4) and at (3/4a, 3/4a, 3/4a), a is the lattice constant. The Sn ions occupy centers of inversion symmetry, but Mg ions do not.

The lattice vibration frequencies are roots of the secular equation

$$|m_k \omega^2 \delta_{kk'} + [\frac{k k'}{\alpha \beta}]| = 0, \quad (1)$$

where $k = 1$ for the Sn core, $k = 1'$ for the Sn shell, and $k = 2$ and 4 for the Mg ions. α and β index the coordinates $x, y,$ and z . The coupling coefficients $[\frac{k k'}{\alpha \beta}]$ are written as the sum of the short range and Coulomb coupling coefficients, $S[\frac{k k'}{\alpha \beta}]$ and $C[\frac{k k'}{\alpha \beta}]$. The Coulomb terms have been tabulated by KELLERMAN⁽²³⁾ and by WHITTEN *et al.*⁽¹⁾ for 47 points in the Brillouin zone. The only difference between $C[\frac{1 k'}{\alpha \beta}]$ and $C[\frac{1 k}{\alpha \beta}]$ is the charge multiplying the coefficient.

We list below the expression of GANESAN and SRINIVASAN⁽²⁴⁾ for the short range coupling coefficients with appropriate changes for our shell model.

$$S[\frac{11}{\alpha \alpha}] = -8\alpha_1 - 4\alpha_2 - 8\beta_2 + 4\alpha_2 \cos \frac{a}{2} q_\beta \cos \frac{a}{2} q_\gamma + 4\beta_2 \cos \frac{a}{2} q_\alpha \left(\cos \frac{a}{2} q_\beta + \cos \frac{a}{2} q_\gamma \right) - \delta, \quad (2)$$

$$S[\frac{11'}{\alpha \beta}] = 4\gamma_2 \sin \frac{a}{2} q_\alpha \sin \frac{a}{2} q_\beta,$$

$$S[\frac{11'}{\alpha \alpha}] = \delta,$$

$$S[\frac{11'}{\alpha \alpha'}] = 0,$$

$$S[\frac{12}{\alpha \alpha}] = \alpha_1 [\exp[i(a/4)(q_\alpha + q_\beta + q_\gamma)] + \exp[i(a/4)(q_\alpha - q_\beta - q_\gamma)] + \exp[i(a/4)(-q_\alpha + q_\beta - q_\gamma)] + \exp[i(a/4)(-q_\alpha - q_\beta + q_\gamma)],]$$

$$S[\frac{12'}{\alpha \beta}] = \beta_1 [\exp[i(a/4)(q_\alpha + q_\beta + q_\gamma)] - \exp[i(a/4)(q_\alpha - q_\beta - q_\gamma)] - \exp[i(a/4)(-q_\alpha + q_\beta - q_\gamma)] + \exp[i(a/4)(-q_\alpha - q_\beta + q_\gamma)],]$$

$$S[\frac{1'2}{\alpha \alpha}] = 0,$$

$$S[\frac{1'2}{\alpha \beta}] = 0,$$

$$S[\frac{1'4}{\alpha \alpha}] = 0,$$

$$S[\frac{1'4}{\alpha \beta}] = 0,$$

$$S[\frac{22}{\alpha \alpha}] = -4\alpha_1 - 2\alpha_3 - 4\beta_3,$$

$$S[\frac{22'}{\alpha \beta}] = 0,$$

$$S[\frac{24}{\alpha \alpha}] = 2\beta_3 \left(\cos \frac{a}{2} q_\beta + \cos \frac{a}{2} q_\gamma \right) + 2\alpha_3 \cos \frac{a}{2} q_\alpha,$$

$$S[\frac{24'}{\alpha \alpha}] = 0,$$

where $\alpha \neq \beta$ and a is the lattice constant. The remaining coefficients can be obtained by the relations

$$S[\frac{k k'}{\alpha \beta}] = S[\frac{k' k}{\beta \alpha}]^*,$$

$$S[\frac{1'4}{\alpha \beta}] = S[\frac{12'}{\alpha \beta}]^*. \quad (3)$$

The subscripts 1, 2, and 3 on the force constants correspond to Mg-Sn, Sn-Sn, and Mg-Mg

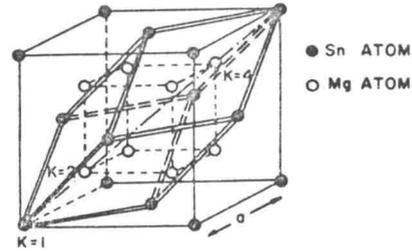


FIG. 6. The crystal structure of Mg₂Sn. The position vectors of the basis in the unit cell are given by $r_k = a/4(k-1)[1, 1, 1]$.

forces, respectively. δ is the force constant associated with the Sn core-Sn shell interaction. (See the appendix for exact definitions of force constants.)

In the limit of long wavelengths ($q = 0$), we have as roots of the secular equation:

$$\omega_A^2 = 0,$$

$$\omega_R^2 = \frac{4}{m_2} (\alpha_1 + \alpha_2 + 2\beta_3),$$

$$\omega_I^2 = \left(\frac{2}{m_1} + \frac{1}{m_2} \right) \left(4\alpha_1 - 2C \frac{e_2^2}{V \left(1 - \frac{4\pi}{3V} \alpha \right)} \right), \quad (4)$$