which are quite similar to the shell model have been discussed in detail.[1,2]

The crystal structure of Mg_2Sn is the same as CaF_2. (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 $(\frac{3}{4}a, \frac{3}{4}a, \frac{3}{4}a)$, 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

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

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 $[{}^{kk'}_{\alpha\beta}]$ are written as the sum of the short range and Coulomb coupling coefficients, $S[{}^{kk'}_{\alpha\beta}]$ and $C[{}^{kk'}_{\alpha\beta}]$. 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 $C[{}^{1k}_{\alpha\beta}]$ and $C[{}^{1k'}_{\alpha\beta}]$ 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.

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

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

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

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

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

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

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

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

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

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

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

$$S[{}^{22}_{\alpha\beta}] = 0,$$

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

$$S[{}^{24}_{\alpha\alpha}] = 0,$$

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

$$S[{}^{kk'}_{\alpha\beta}] = S[{}^{k'k}_{\beta\alpha}]^*,$$
$$S[{}^{14}_{\alpha\beta}] = S[{}^{12}_{\alpha\beta}]^*. \qquad (3)$$

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

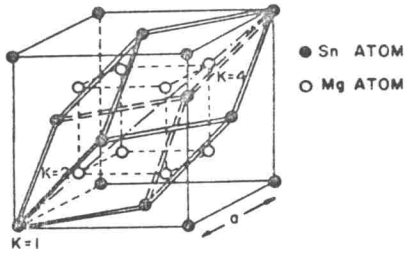

FIG. 6. The crystal structure of Mg_2Sn. The position vectors of the basis in the unit cell are given by $r_k = a/4(k-1)[1, 1, 1]$.

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:

$$\omega_A^2 = 0,$$

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

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