

Figure 2-13 Dispersion curves for diamond. Data from J. L. Warren, R. G. Wenzel and J. L. Yamell, *Inelastic Scattering of Neutrons* (Vienna, International Atomic Energy Agency, 1965).

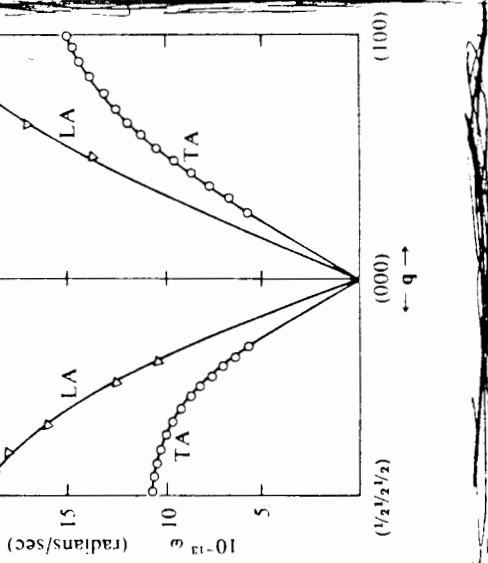


FIG. 1. Dispersion curves for gallium arsenide based on measurements at 296°K. The solid points denote undetermined polarization. The vertical dashed line in the $[001]$ direction represents the zone boundary. In this direction, points labeled I, II refer to modes whose polarization vectors are parallel to the (011) mirror plane. Other modes are either strictly longitudinal (L) or transverse (T). The dotted and solid curves represent calculations based on two modifications, B and C, of the dipole approximation model.

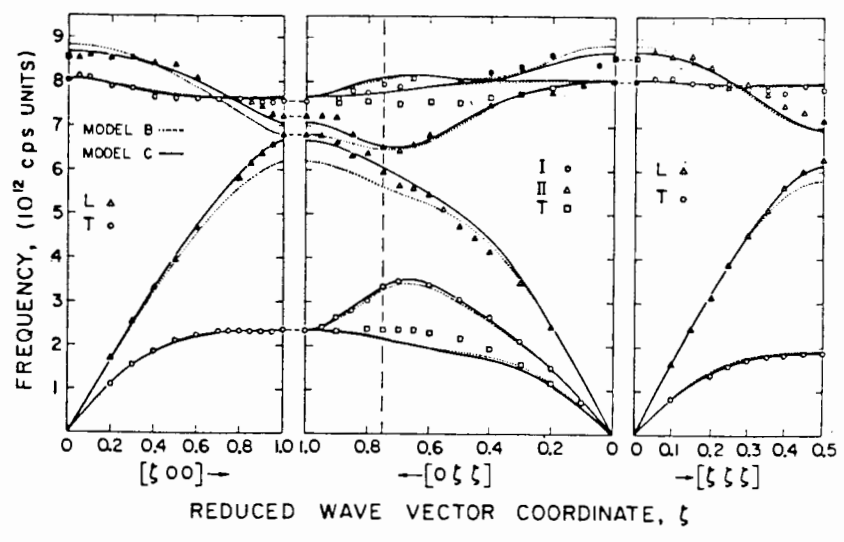


FIG. 1. Dispersion curves for diamond, silicon, and germanium in dimensionless units. If the three elements were homologous, the curves should coincide. The solid lines were calculated from the elastic constants of diamond given by McSkimin and Bond

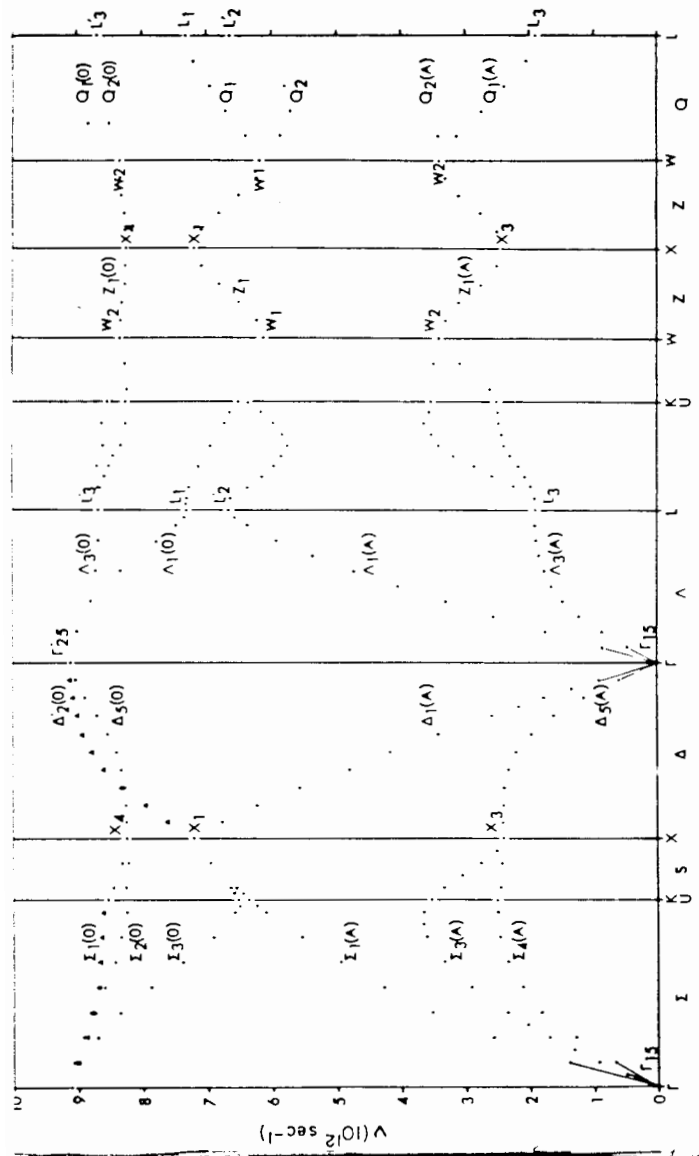
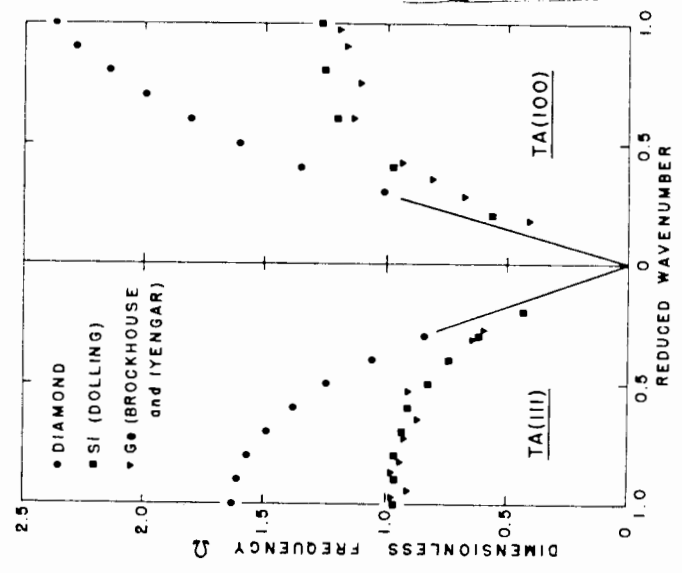


FIG. 2. Measured phonon dispersion relations in Ge at 80°K.

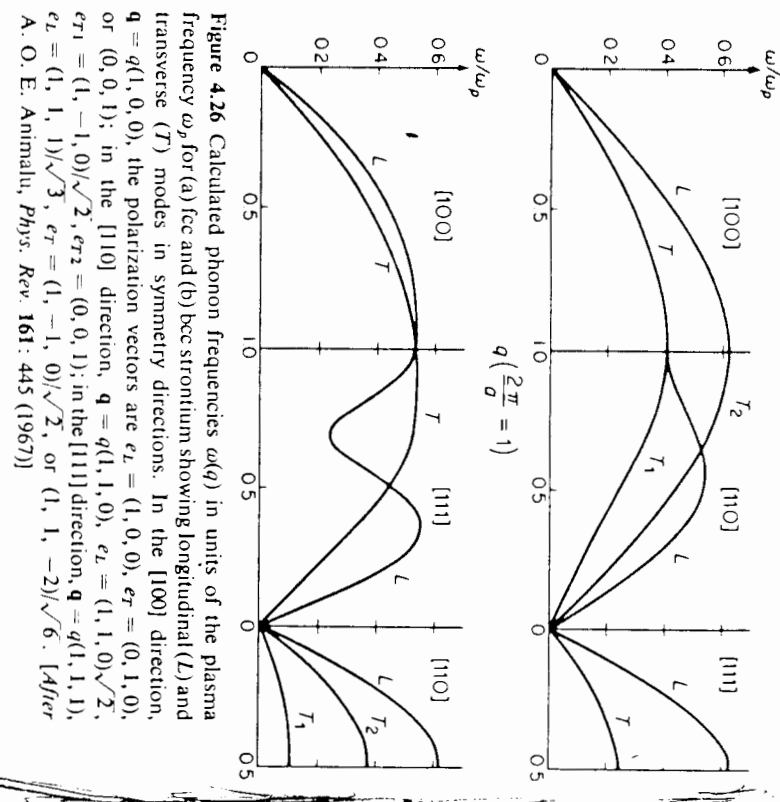


Figure 4.26 Calculated phonon frequencies $\omega(q)$ in units of the plasma frequency ω_p for (a) fcc and (b) bcc strontium showing longitudinal (L) and transverse (T) modes in symmetry directions. In the $[100]$ direction, $\mathbf{q} = q(1, 0, 0)$, the polarization vectors are $e_L = (1, 0, 0)$, $e_T = (0, 1, 0)$, or $(0, 0, 1)$; in the $[110]$ direction, $\mathbf{q} = q(1, 1, 0)$, $e_L = (1, 1, 0)/\sqrt{2}$, $e_{T1} = (1, -1, 0)/\sqrt{2}$, $e_{T2} = (0, 0, 1)$; in the $[111]$ direction, $\mathbf{q} = q(1, 1, 1)$, $e_L = (1, 1, 1)/\sqrt{3}$, $e_T = (1, -1, 0)/\sqrt{2}$, or $(1, 1, -2)/\sqrt{6}$. [After A. O. E. Animalu, *Phys. Rev.* **161**: 445 (1967)]

LiF

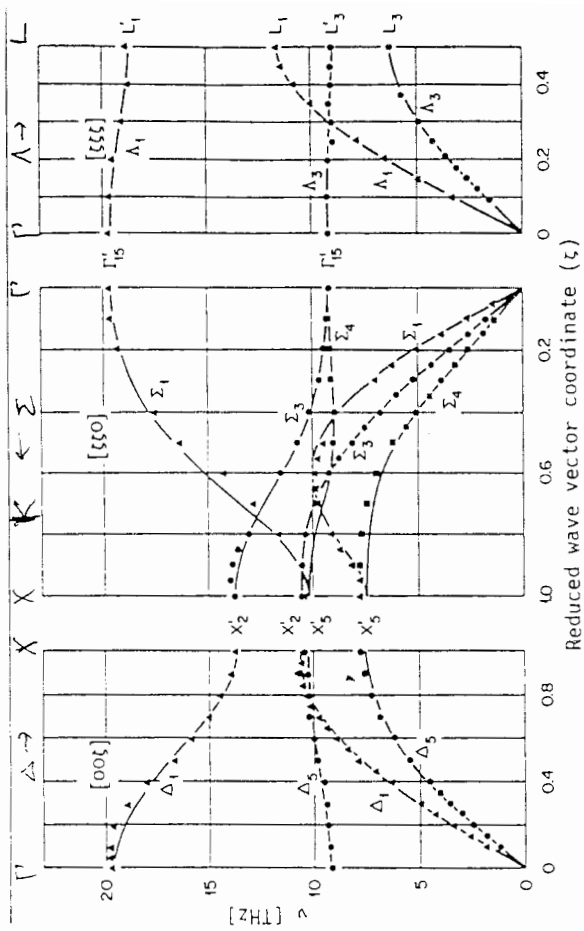


Fig. 4.2a. LiF: $\omega(q)$ [Ref. 4, 10, Fig. 4], $T = 298$ K, M: 7P-SM, Lit. [4, 2, 11-13, 64]

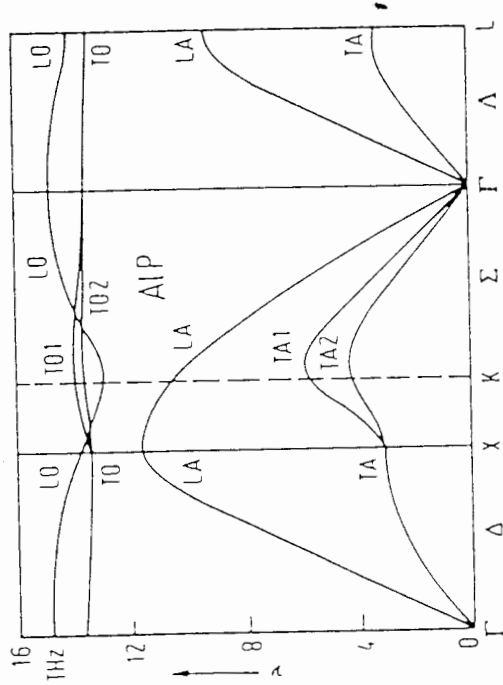


Fig. 3. AIP. Phonon dispersion relations [85K I].

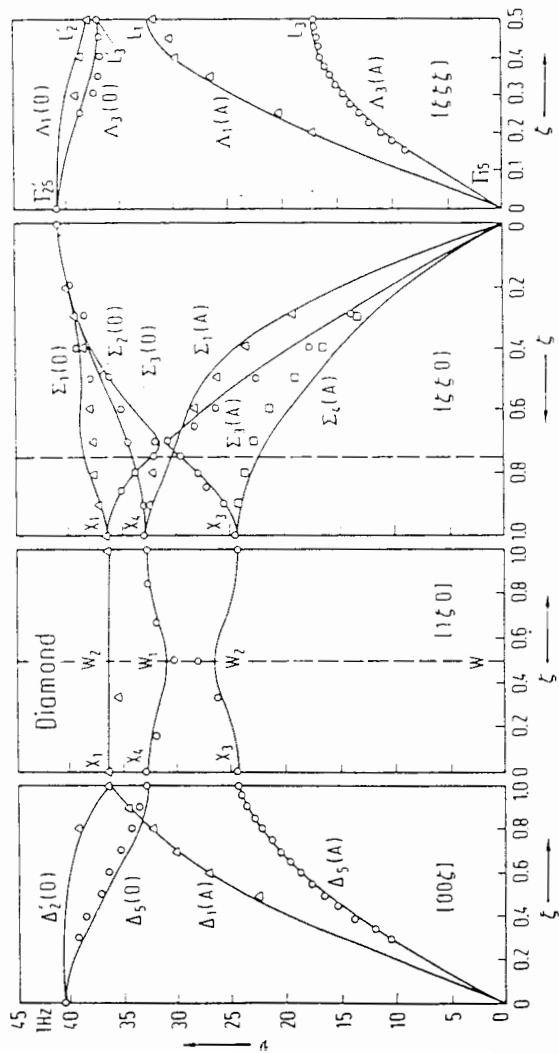


Fig. 6. Diamond. Phonon dispersion relations. Experimental data from neutron scattering, full curves: shell model calculation [67W].

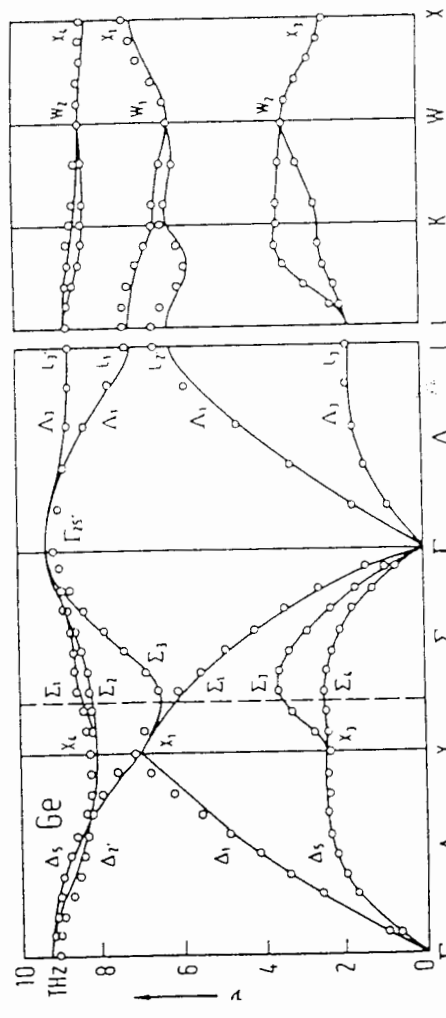


Fig. 7. Ge. Phonon dispersion relations. Experimental points from [71N, 72NI], solid lines: theory [77W].

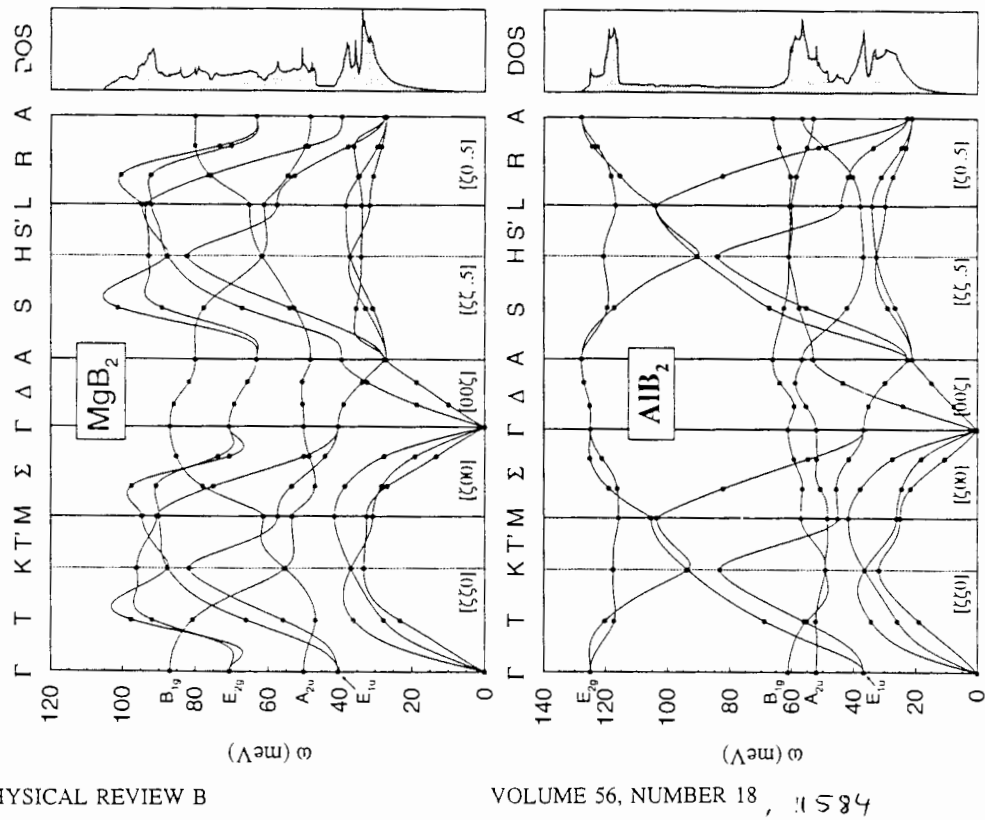


FIG. 2. Theoretical phonon dispersion curves along high-symmetry lines of the hexagonal BZ (notation after [32]) and DOS of MgB_2 and AIB_2 . The dots represent actually calculated modes; lines are obtained by Fourier interpolation.

PHYSICAL REVIEW B

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Lattice dynamics of xenotime: The phonon dispersion relations and density of states of $LuPO_4$

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TABLE IV. Correlation for symmetry species of the T_d group of the PO_4^{3-} free ion, the D_{2d} group of the Lu^{3+} and PO_4^{3-} sites in the $LuPO_4$ crystal, and the D_{4h} group of the whole crystal.

$LuPO_4$ Crystal (D_{4h})	PO_4^{3-} Site Symmetry (D_{2d})	Free PO_4^{3-} Molecule (T_d)	Description of Mode
B_{1g}	B_2	F_2	antisymmetric P-O bond stretch
A_{2u}			
E_g	E	F_2	antisymmetric P-O bond stretch
A_{1g}			
E_u	A_1	A_1	symmetric P-O bond stretch
B_{2u}			
B_{1g}	B_2	F_2	antisymmetric O-P-O bond bend
A_{2u}			
E_g	E	F_2	antisymmetric O-P-O bond bend
B_{2u}			
E_u	A_1	E	symmetric O-P-O bond bend
A_{1g}			
A_{1u}	B_1	E	symmetric O-P-O bond bend
E_u			
B_{1g}	B_1	E	symmetric O-P-O bond bend
B_{2g}			
E_g	B_1	E	symmetric O-P-O bond bend
A_{2u}			
A_{2g}	B_1	E	symmetric O-P-O bond bend
E_u			
E_g	B_1	E	symmetric O-P-O bond bend
E_g			
B_{1g}	B_1	E	symmetric O-P-O bond bend
E_g			
B_{1u}	B_1	E	symmetric O-P-O bond bend
B_{1u}			
			translation-like or rotation-like

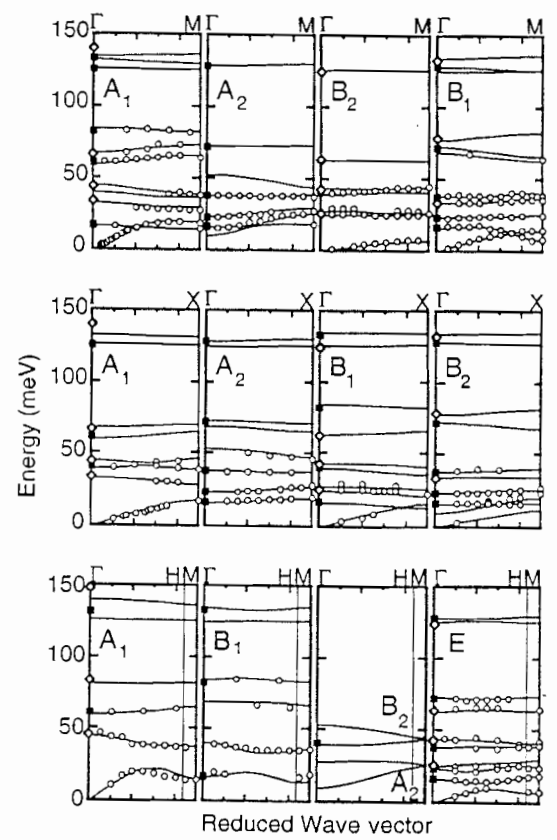


FIG. 4. Phonon-dispersion curves of $LuPO_4$ along the $[x,0,0]$, $[x,x,0]$, and $[0,0,x]$ symmetry directions. The symbols (\blacksquare = Raman, \diamond = Infrared, and \circ = neutron) indicate observed data, while the lines are calculated using the lattice dynamics model.