

ESEMPI ILLUSTRATIVI DELLE CURVE DI DISPERSIONE FONONICA

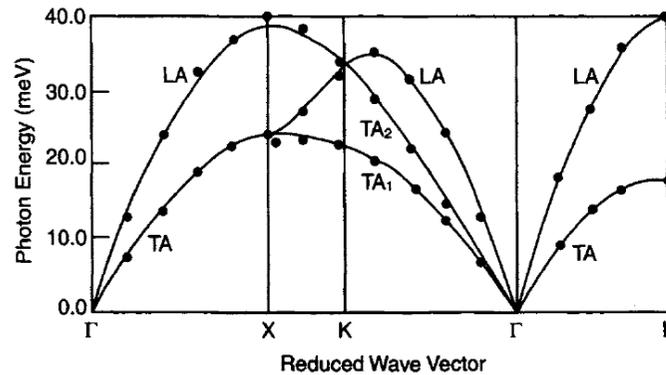


Fig. 5 Phonon dispersion curves of aluminum along symmetry directions. The solid lines represents the calculations of A. A. Quong and B. M. Klein, Phys. Rev. B46, 10734 (1992) (copyright 1992 by the American Physical Society). Longitudinal and transverse acoustic branches are indicated by LA and TA (or TA₁ and TA₂), respectively. The experimental points are from the papers of G. Gilat and R. M. Nicklow, Phys. Rev. 143, 487 (1966) and R. Stedman, S. Almqvist and G. Nilsson, Phys. Rev. 162, 549 (1967).

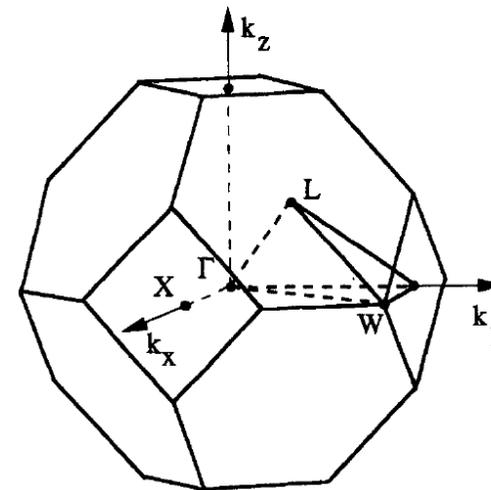
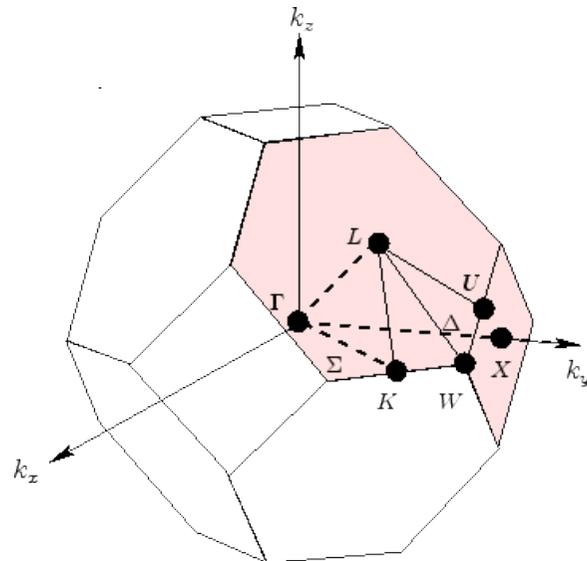


Fig. 18 Brillouin zone for the face-centered cubic lattice (truncated octahedron). Some high symmetry points are: $\Gamma = 0$; $X = (2\pi/a)(1, 0, 0)$; $L = (2\pi/a)(1/2, 1/2, 1/2)$; $W = (2\pi/a)(1/2, 1, 0)$.

Si e Ge : fcc base 2. Notare a sinistra delle curve la densità degli stati

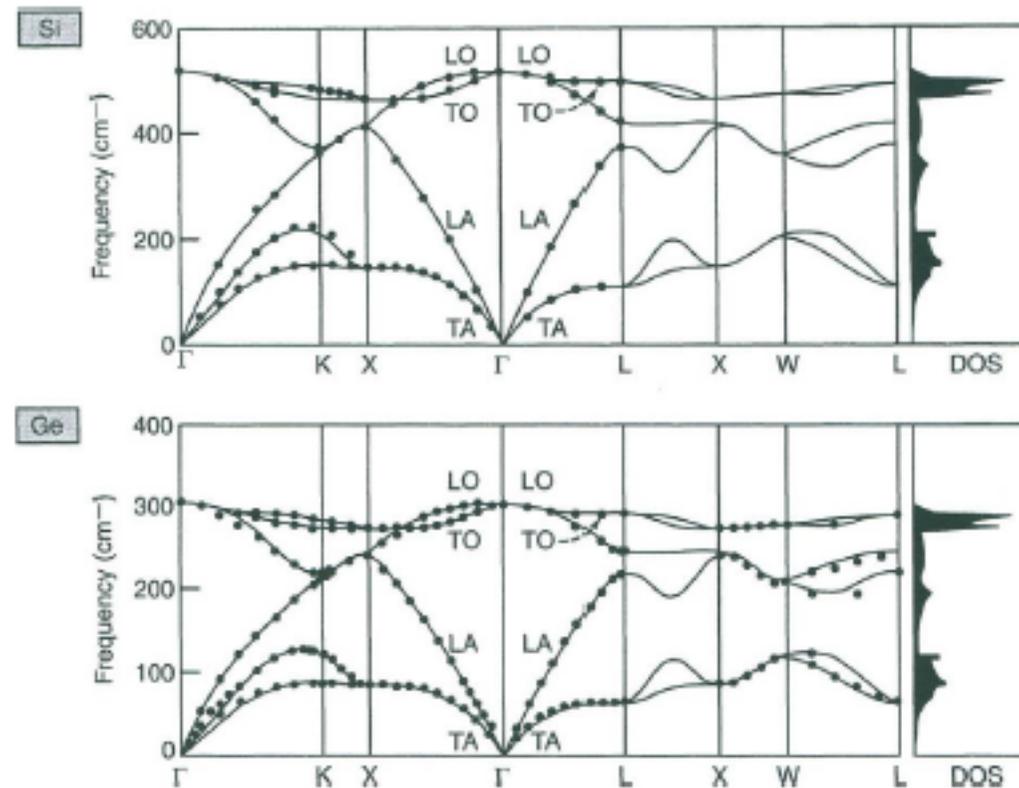


Fig. 6 Phonon dispersion curves and density-of-states of Si and Ge calculated by P. Gianozzi, S. de Gironcoli, P. Pavone and S. Baroni, Phys. Rev. B43, 7231 (1991) (copyright 1991 by the American Physical Society). Longitudinal and transverse acoustic (or optical) modes are indicated by LA and TA (LO and TO), respectively. The experimental points are from G. Dolling, in "Inelastic Scattering of Neutrons in Solids and Liquids" edited by S. Eklund (IAEA, Vienna 1963) Vol.II, p.37; G. Nilsson and G. Nelin, Phys. Rev. B3, 364 (1971) and Phys. Rev. B6, 3777 (1972). Conversion to meV units can be done noting that $1 \text{ cm}^{-1} = 0.124 \text{ meV}$.

Semiconduttori : fcc con 2 atomi per cella unitaria. Notare a sinistra delle curve la densità degli stati. Il legame chimico e' parzialmente ionico. La differenza di massa degli atomi nella cella unitaria e' grande quindi branche ottiche ed acustiche sono ben separate

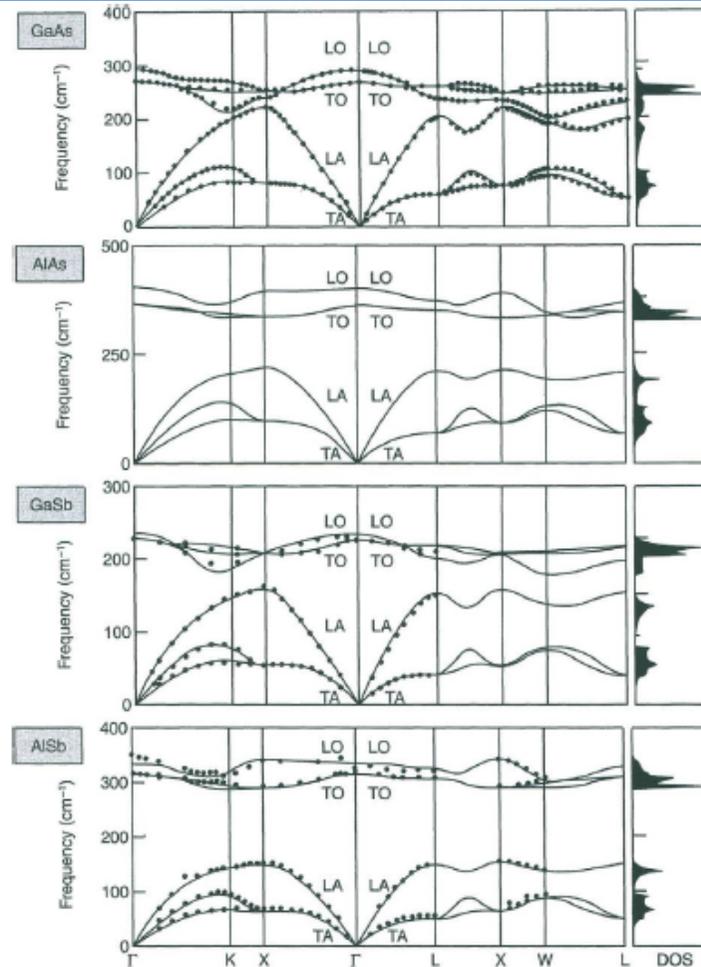


Fig. 7 Calculated phonon dispersion curves and density-of-states for binary semiconductors GaAs, AlAs, GaSb and AlSb [from P. Giannozzi, S. de Gironcoli, P. Pavone and S. Baroni, Phys. Rev. B **43**, 7231 (1991); copyright 1991 by the American Physical Society]. Longitudinal and transverse acoustic (or optical) modes are indicated by LA and TA (LO and TO), respectively.

LiF fcc base 2.

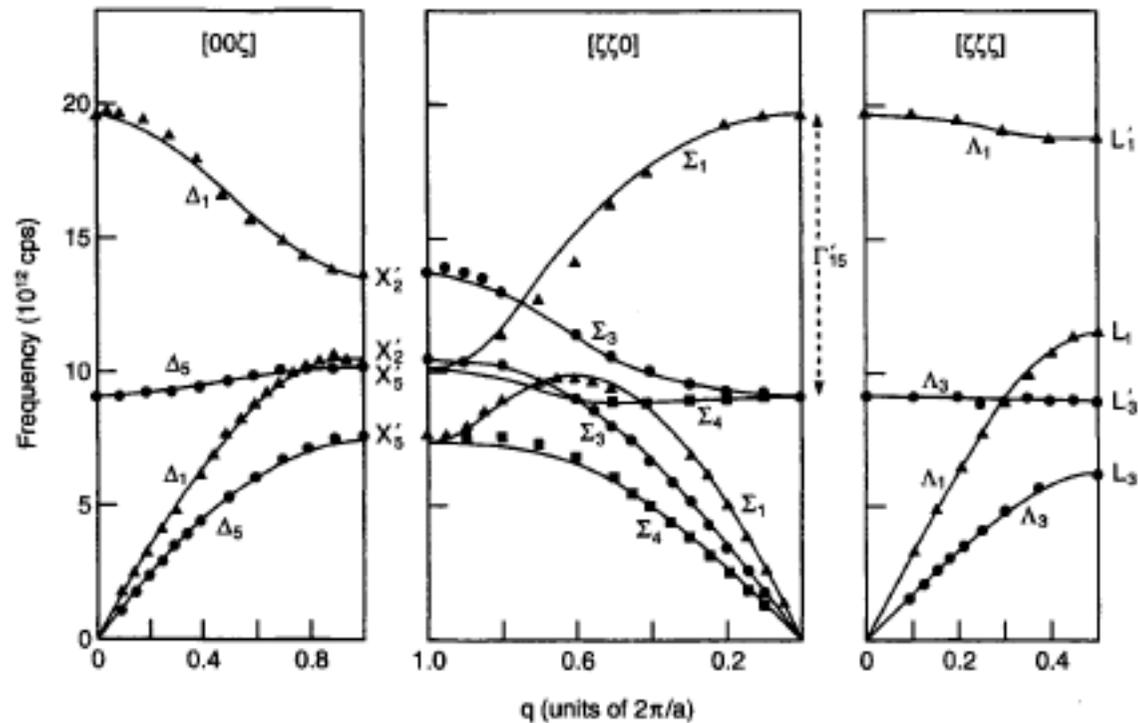
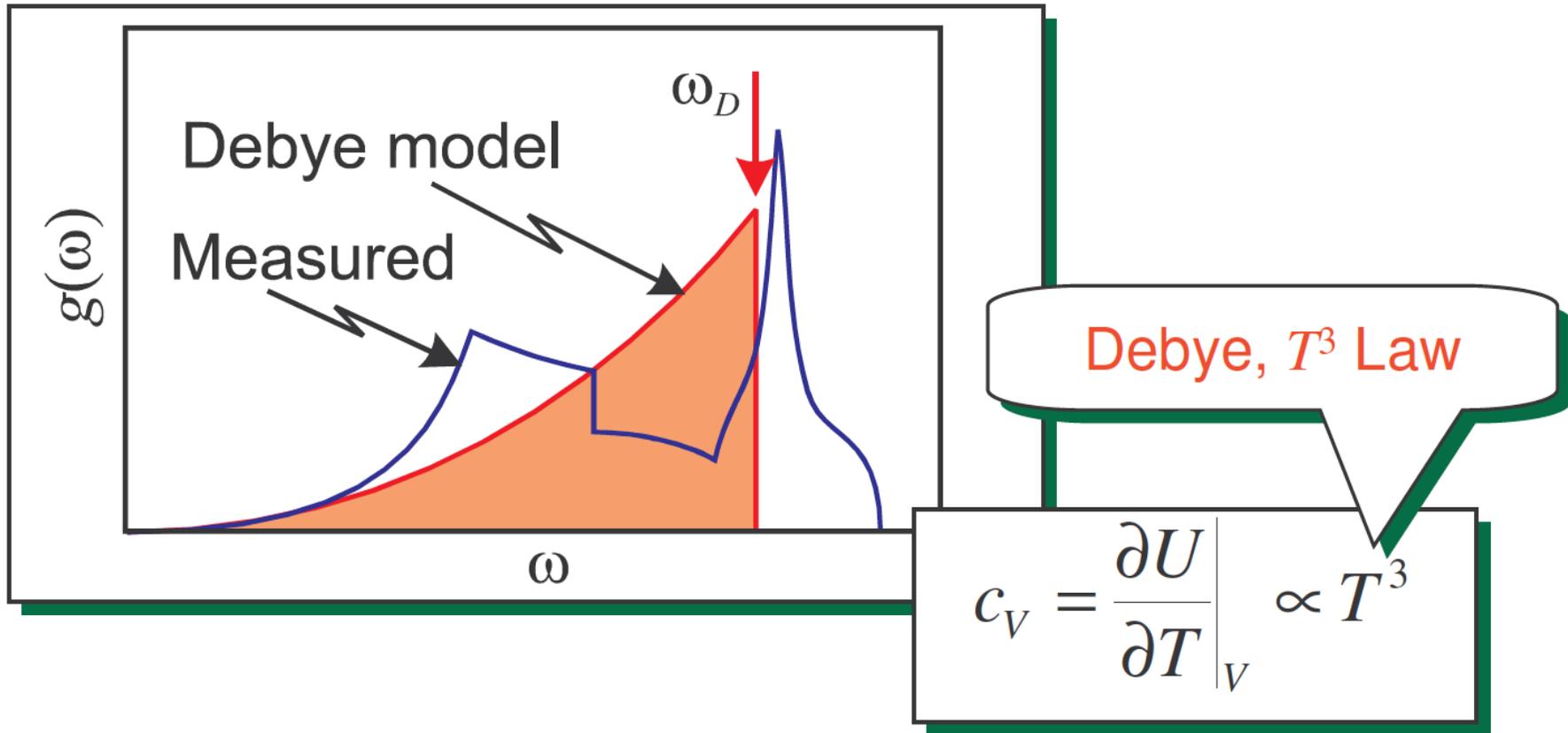


Fig. 8 Measured phonon dispersion curves along three directions of high symmetry in LiF; the solid curves are a best least-squares fit of a parameter model [from G. Dolling, H. G. Smith, R. M. Nicklow, P. R. Vijayaraghavan and M. K. Wilkinson, *Phys. Rev.* **168**, 970 (1968); copyright 1968 by the American Physical Society].

DOS $D(\omega)$ per l'alluminio e approssimazione di Debye
A bassa T va bene



Predizioni Debye e Einstein per il rame ed esperimento

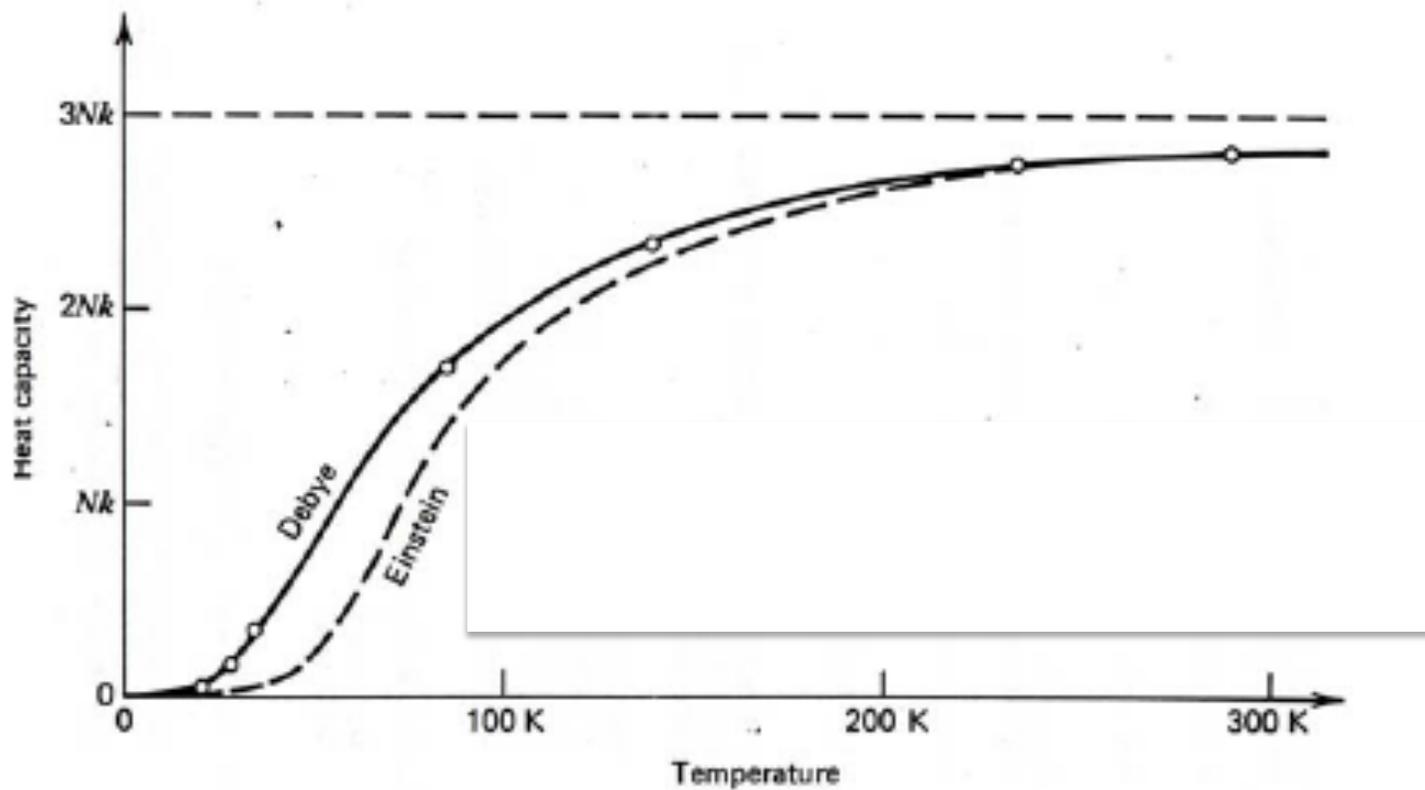


Figure 27.12 Comparison of Einstein and Debye model predictions with data for the heat capacity of copper.