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On Van Hove Singularities in Pure Cubic Crystals AZITA JOVAINI, JAMES PIENTKA, SHIGEJI FUJITA, University at Buffalo, SALVADOR GODOY, UNAM, AKIRA SUZUKI, Tokyo University of Science — Pure elements form crystals of various lattices, cubic, tetragonal and others. At very low temperatures the lattice heat capacities in three dimensional crystals obey Debye's T^3-law, where T is the absolute temperature. X-ray scattering experiments and lattice dynamics calculations reveal van Hove singularities when the density of states is plotted as a function of the phonon frequency. A physical origin of the singularities, jumps in the derivative of the density of states, is clarified. The singularities occur in three and two dimensions when the constant-frequency plane touches the Brillouin zone boundary *and* undergoes a curvature inversion. The face-centered cubic lattice is composed of two simple cubic sublattices and one tetragonal sublattice. The first (second) major peaks in the observed density of states in aluminum (Al) are shown to arise from the transverse phonons associated with the cubic (tetragonal) sublattices. We predict that the density of states has one major peak with a shoulder (two peaks with shoulders) for a body-centered cubic (face-centered cubic) crystal.

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