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Heat Capacity and Isotopic Masses of Semiconductors MANUEL CARDONA, REINHARD K. KREMER, GISELA SIEGLE, RUDOLF LAUCK, MPI-FKF, JORGE SERRANO, ESRF, ALDO H. ROMERO, CINVESTAV, Querétaro, México — The heat capacity of semiconductors has been investigated both theoretically and experimentally since the early 20^{th} century. Its dependence on the isotopic masses of its constituents, however, has only received attention during the past few years [1]. The quantity usually investigated vs. temperature$T$is D(T)= d ln $C_v T^{-3}$ / d ln M.For monatomic diamond, Si, and Ge, D(T) exhibits a peak at a temperature 0.1 times that of TA phonons at the X-point of the BZ. In binary tetrahedral semiconductors (GaN, ZnO) D(T) differs for the heavier and lighter mass, peaking at 0.15 times the TA temperature of the former and at 0.25 times the TO temperature of the latter. The ratio 0.15 can also can also be estimated with a one-oscillator Einstein model. Here we present similar measurements for a binary compound with rock salt structure: PbS (galena). The phonon density of states (DOS) of this material is shown to peak at 80K for the Pb-like phonons. For the S-like phonons a broad band between 150 and 350K is found, in *ab initio* calculations, to dominate the DOS. The corresponding D(T) peaks in both cases at 0.14 times the temperature of the corresponding phonons (80K and 240K, respectively). The D(T) will be compared with *ab initio* calculations, performed with the ABINIT code. [1] J.Serrano, Phys. Rev. B 73, 094303 (2006) and references therein.

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