Empirical Relation between Energy Gap and Lattice Constant in Cubic Semiconductors

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The empirical relation $E_0 \propto (1/a_0^2)$ between the energy gap E_0 and lattice constant a_0 has been found to hold for a wide range of semiconductors with the cubic NaCl crystal structure.

In a previous letter,[1] an empirical relation between the energy gap E_0 and lattice constant a_0 of cubic (NaCl structure) semiconductors was applied to PbS, PbSe, PbTe, and PbPo. This relation, which states that E_0 is directly proportional to $1/a_0^2$ for a series of related semiconductors, was known[2] to hold reasonably well for the group-IV elemental semiconductors. The purpose of this addendum is to show that this empirical relation holds for a large number of semiconductors with the NaCl fcc crystal structure.

Values[3] of energy gap E_0 were plotted as a function of $1/a_0^2$ for the following sequences of related semiconductors: (1) BaS, BaSe, BaTe; (2) CaS, CaSe, CaTe; (3) SrS, SrSe, SrTe; (4) solid solutions of SnTe in PbTe; (5) solid solutions of SnSe in PbSe. The results for sequences (1)–(4) are shown in Figs. 1 and 2; the result for sequence (5) is shown in the letter[1] mentioned above.

For all five sequences of semiconductors with the NaCl structure, the empirical relation E_0

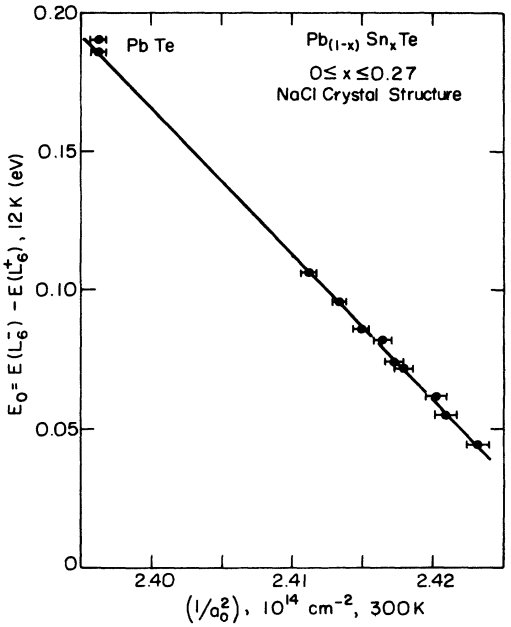

FIG. 2. Energy gap E_0 plotted as a function of $1/a_0^2$ for solid solutions of SnTe in PbTe.

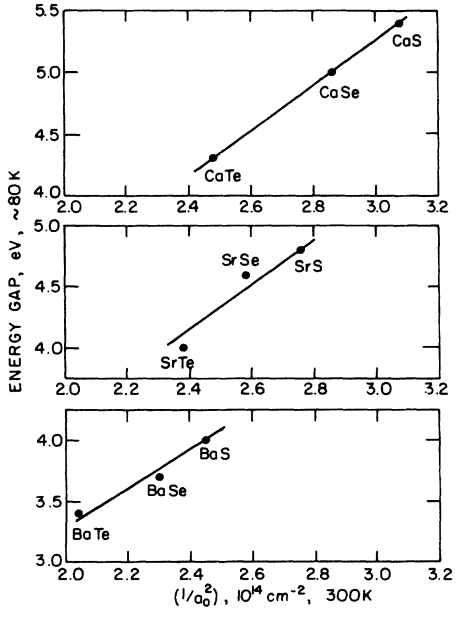

FIG. 1. Energy gap plotted as a function of $1/a_0^2$ for CaS, CaSe, CaTe; SrS, SrSe, SrTe; BaS, BaSe, BaTe.

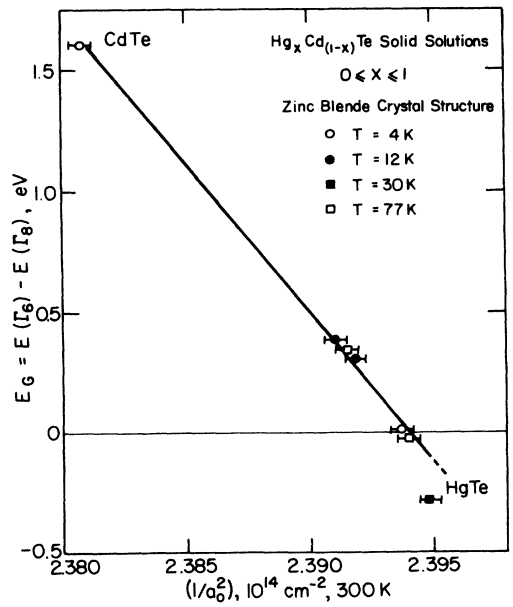

FIG. 3. Energy gap $E_G \equiv E(\Gamma_6) - E(\Gamma_8)$ plotted as a function of $1/a_0^2$ for solid solutions of HgTe in CdTe.

$\propto 1/a_0^2$ is well satisfied. It is of particular interest that the data for solid solutions of SnSe in PbSe cover both positive and negative values of $E_0 \equiv E(L_6^-) - E(L_6^+)$. For this reason, it is also of interest to note that this empirical relation holds also for CdTe,[4] for HgTe,[5] and for solid solutions[6-9] $Hg_{(1-x)}Cd_xTe$ ($0.86 \geq x \geq 0.63$, zinc-blende structure) with both positive and negative values of the energy gap $E_G \equiv E(\Gamma_6) - E(\Gamma_8)$. This result is shown in Fig. 3.

In summary, this empirical relation $E_0 \propto 1/a_0^2$ has been found to hold for a wide range of semiconductors with the NaCl structure with both positive and negative energy gaps. This result has been used, in results published elsewhere,[1,10] to investigate the PbS group of semiconductors, including lead polonide (PbPo).

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