Title
HIGH RESOLUTION TRANSMISSION ELECTRON MICROSCOPY

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Publication Date
1973-08-01

Submitted to Industrial Research

LBL-2219
Preprint c. 1

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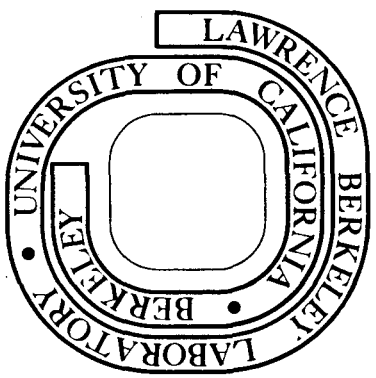
August 1973

Prepared for the U. S. Atomic Energy Commission
under Contract W-7405-ENG-48



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EMPIRICAL RELATION BETWEEN ENERGY GAP AND LATTICE CONSTANT IN CUBIC SEMICONDUCTORS

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ABSTRACT

The empirical relation $E_o \alpha (1/a_o^2)$ between the energy gap E_o and lattice constant a_o 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_o and lattice constant a_o of cubic (NaCl structure) semiconductors was applied to PbS, PbSe, PbTe, and PbPo. This relation, which states that E_o is directly proportional to $(1/a_o^2)$ 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 f.c.c. crystal structure.

Values[3] of energy gap E_o were plotted as a function of $(1/a_o^2)$ 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 Figures 1 and 2 below; 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 $E_o \alpha (1/a_o^2)$ 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 $E_o \equiv E(L_6^-) - E(L_6^+)$. 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 Figure 3.

In summary, this empirical relation $E_o \alpha (1/a_o^2)$ 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).

ACKNOWLEDGEMENT

The author would like to thank the Department of Physics of the University of California, Berkeley, for its hospitality. The generous assistance of the Inorganic Materials Research Division of the Lawrence Berkeley Laboratory is also acknowledged.

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FIGURE CAPTIONS

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

Figure 2. Energy gap E_o plotted as a function of $(1/a_o^2)$ for solid solutions of SnTe in PbTe.

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

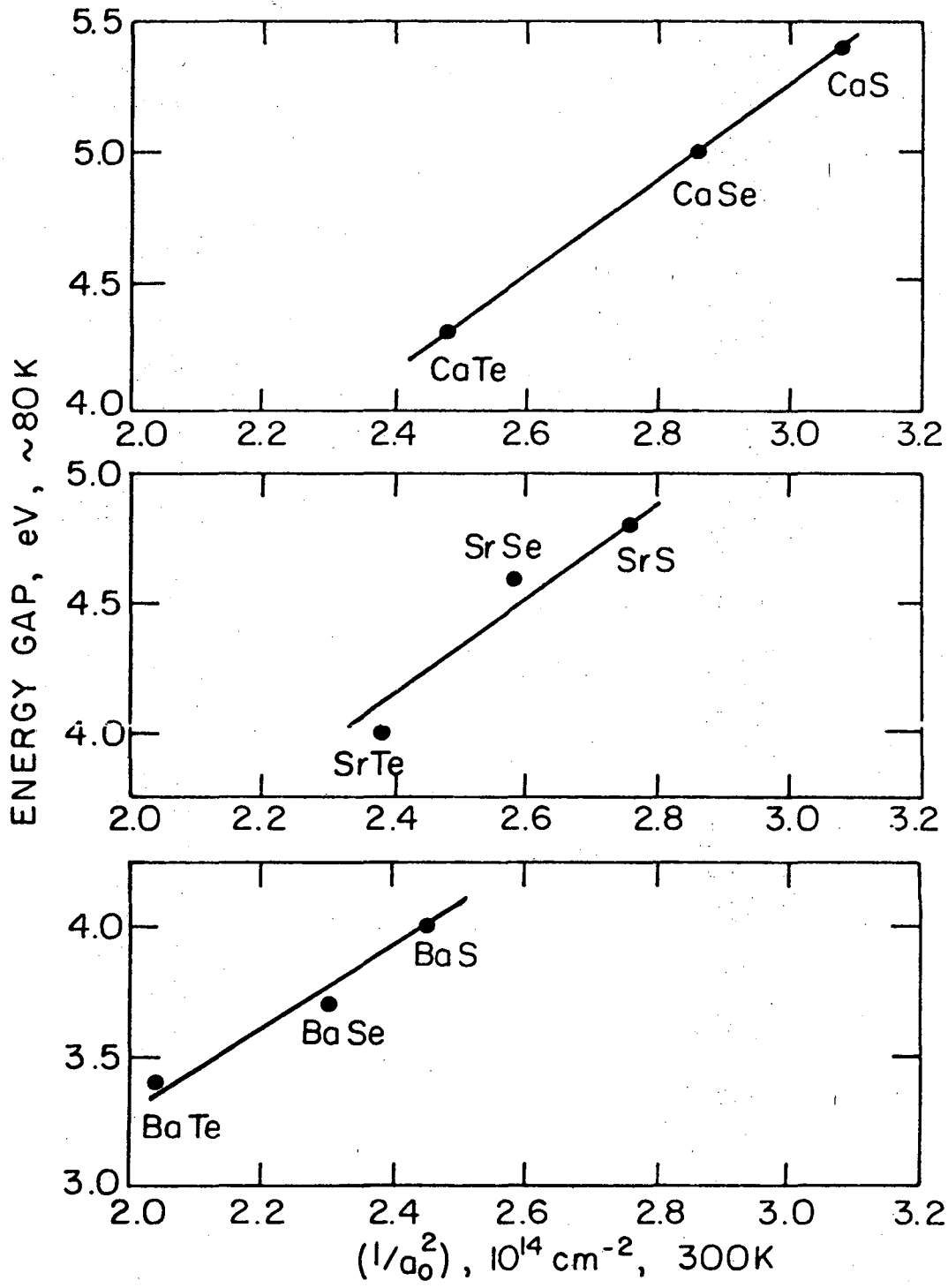

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Fig. 1

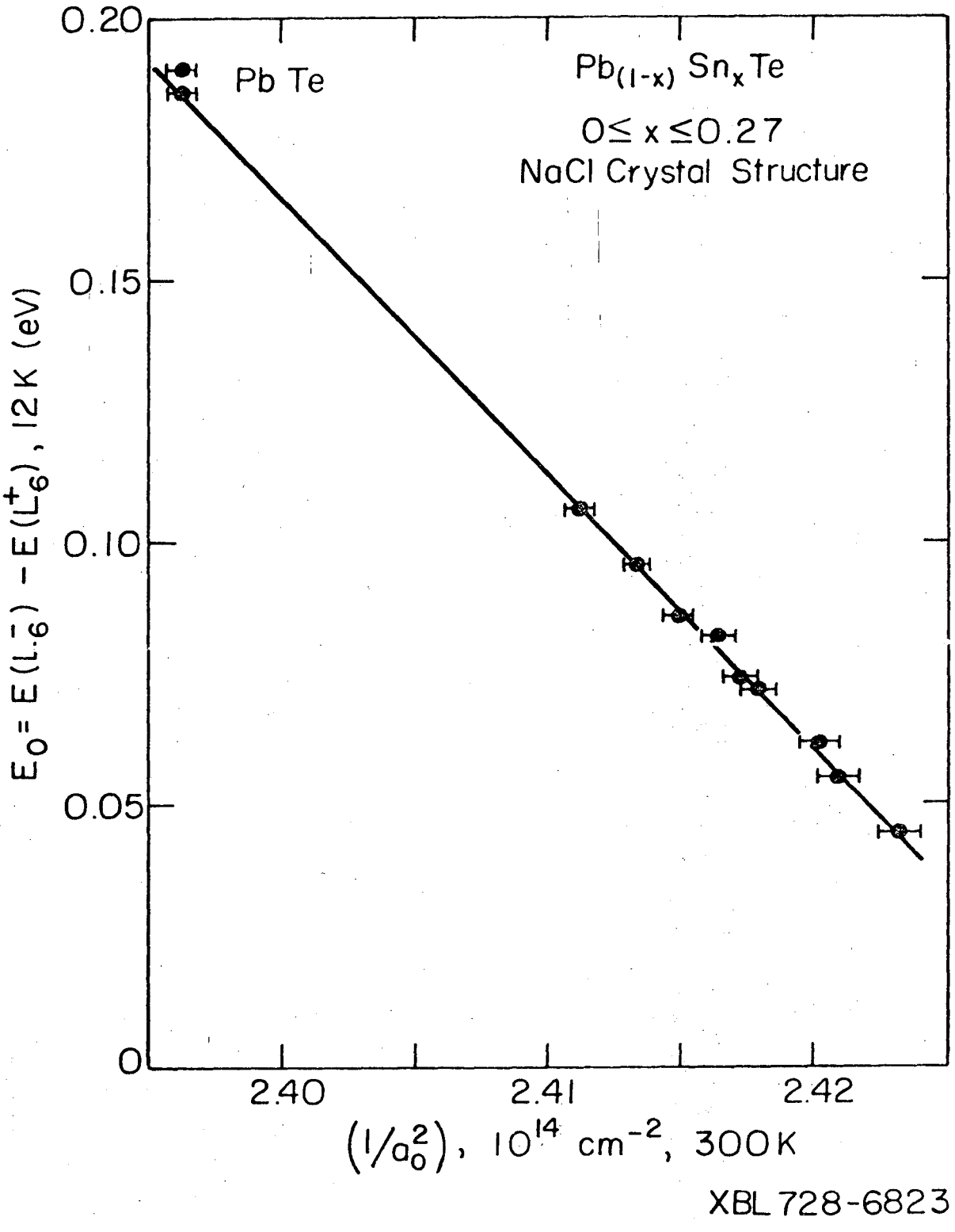
0.20
0.15
0.10
0.05
0
Pb Te
$Pb_{(1-x)}$ Sn_x Te
$0 \leq x \leq 0.27$
NaCl Crystal Structure
$E_0 = E(L_6^-) - E(L_6^+)$, 12 K (eV)
2.40
2.41
2.42
$(1/a_0^2)$, 10^{14} cm^{-2}, 300 K
XBL 728-6823

Fig. 2

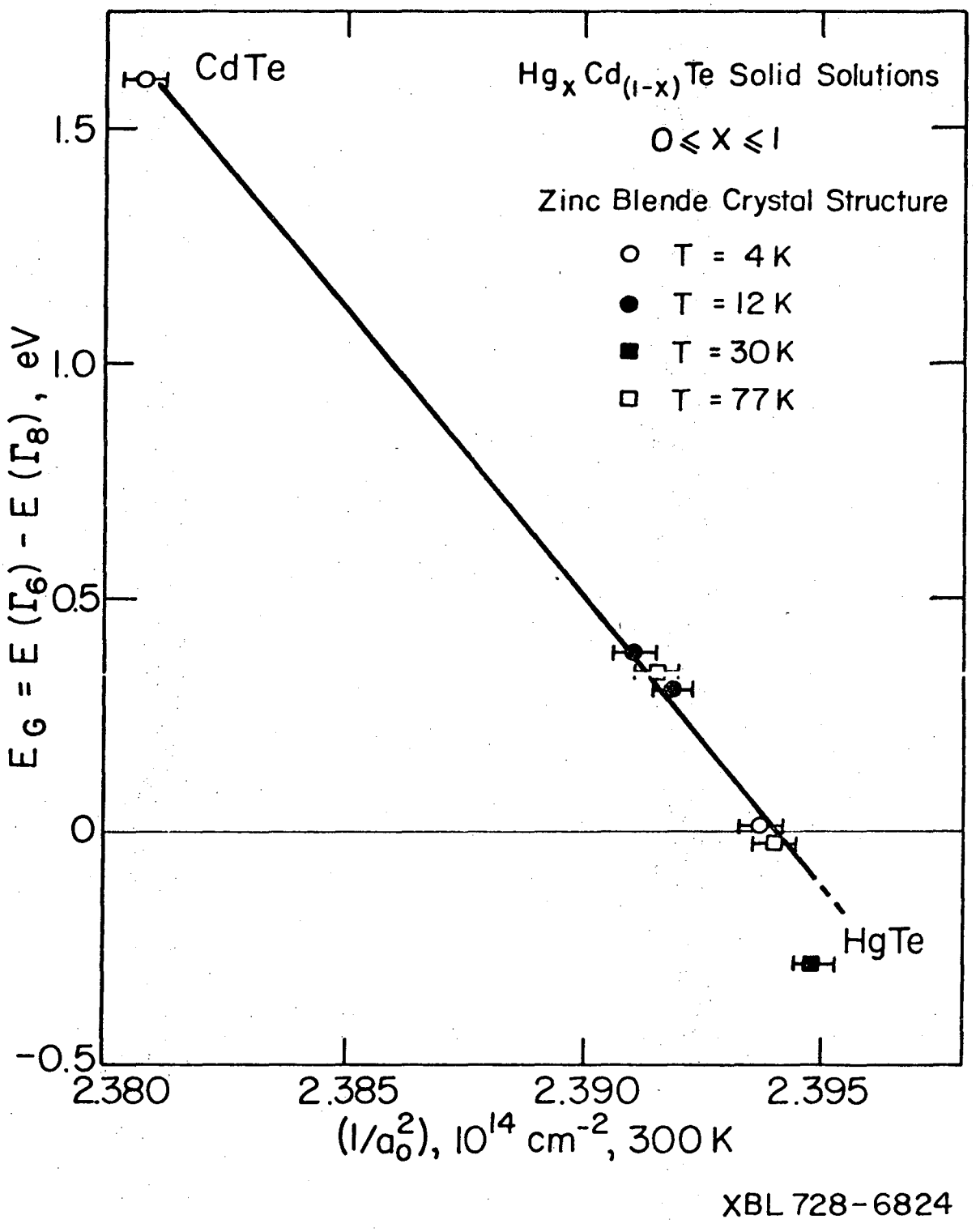
CdTe
$Hg_x Cd_{(1-x)} Te$ Solid Solutions
$0 \leqslant X \leqslant 1$
Zinc Blende Crystal Structure
T = 4 K
T = 12 K
T = 30 K
T = 77 K
HgTe
1.5
1.0
0.5
0
-0.5
$E_G = E(\Gamma_6) - E(\Gamma_8)$, eV
2.380
2.385
2.390
2.395
$(1/a_0^2)$, 10^{14} cm^{-2}, 300 K
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Fig. 3

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