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Submitted to Physical Review Letters

LBL-3900
Preprint c. 1

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April 1975

Prepared for the U. S. Energy Research and Development Administration under Contract W-7405-ENG-48

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Parity Assignments at L in the Lead Salt Semiconductors

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ABSTRACT

It is concluded that the results of Glosser et al (Phys. Rev. Letters 33, 1027 (1974)) do not require new parity assignments for the bands at L in PbTe.

In a recent Letter[1], Glosser et al have concluded that the accepted parity assignments[2] of the bands at L are incorrect for PbTe. The purpose of this Comment is to suggest that the conclusion of Glosser et al is not justified.

The currently accepted parity assignments at L (given by Martinez et al[2]) are shown in Table I, as is the scheme proposed by Glosser et al. The parity

Table I: Parity Assignments at L

Band	PbTe (A)[a]	PbTe (G)[b]	PbSe (A)[a]	PbSe (G)
L(8)	L_6^-	L_6^+	L_{45}^-	L_{45}^+
L(7)	L_{45}^-	L_{45}^+	L_6^-	L_6^+
L(6) = CB	L_6^-	L_6^-	L_6^-	L_6^-
L(5) = VB	L_6^+	L_6^+	L_6^+	L_6^+
L(4)	L_{45}^+	L_{45}^-	L_{45}^+	L_{45}^-
L(3)	L_6^+	L_6^-	L_6^+	L_6^-

a = Reference 2 (A = "accepted"); b = Reference 1 (G = Glosser et al); VB = highest valence band; CB = lowest conduction band.

assignments for PbTe labeled (G) in Table I are those proposed by Glosser and are a set of assignments in which the parities of the band edges [L(5), L(7), L(8)] and of [L(3), L(4), L(6)] are the same. This scheme was explicitly proposed

for PbTe[1]. Since the only difference between bands L(3) through L(8) in PbTe and in PbSe is the relative ordering of L(7) and L(8), then, if Glosser's proposed parity assignments are correct for PbTe, they should also be correct for PbSe. The accepted[2] (A) assignments for PbSe are shown in Table I, as is the set of assignments (G) implied for PbSe by Glosser's proposed assignments for PbTe.

It is known experimentally[3] that, for PbTe, the valence band (L(5)) edge wave function has a strong s-like character, thereby establishing an L_6^+ valence band edge for PbTe. it is also known that the conduction band (L(6)) edge is an L_6^- state. Further, these state are also the case for the L(5) and L(6) bands in PbSe and PbS. This is known to be true because two binary alloys[4] of the three lead salts do <u>not</u> exhibit the vanishing of the energy gap seen in PbTe-SnTe and PbSe-SnSe solid solutions, so the band gap states of PbSe and PbS are <u>not</u> inverted relative to those in PbTe.

With the parity assignments for L(5) and L(6) known from experiment, the two arrangements of bands labeled (G) in Table I are the only ones which exhibit the features proposed by Glosser in his alternate scheme of parity assignments.

The evidence put forth by Glosser[1] is basically the non-observation of a critical point transition at L under circumstances (i.e., the Fermi level out of the band) under which one would expect to observe only critical point transitions. This null result is interpreted as meaning that the transition is forbidden because the initial and final state at L have the same parity.

It appears to the author that this conclusion is based on equating the Laporte selection rule[5] with its converse. This rule states that, under certain circumstances, matrix elements of the electric dipole moment operator vanish unless the initial and final states have opposite parities. It seems unjustified to use the

converse of this selection rule to conclude that the non-observation of a transition means, first, that it is forbidden, and that, second, it is forbidden because of the parity selection rule mentioned above. It may simply be the case that the electric dipole matrix element for the transition in question is small, but not zero, so the transition is merely relatively weak, and not forbidden.

Glosser does not mention explicitly which non-observed transition(s) he is considering. Form the photon energy range (about 1.2 - 2.0 eV) quoted in his Letter, it appears that he is dealing with the L(5 → 7), i. e., $L_6^+ \rightarrow L_{45}^-$, transition (using the accepted parity labels). If Glosser's parity assignments, as given in Table I, are correct for PbTe, then L(5 → 7) would be an $L_6^+ \rightarrow L_{45}^+$ transition, and would be forbidden[6] by the parity selection rule. However, it should again be noted that this new set of parity labels for PbTe would imply the parity assignments labeled (G) in Table I for PbSe. This in turn would imply that the L(5 → 7) and L(4 → 6) electric dipole transitions in PbSe would be forbidden and hence not observed. However, both of these transitions have been observed[7,8] in modulated reflectivity experiments on PbSe, although not in similar experiments on PbTe.

For these reasons, it appears to the author that Glosser et al's results on PbTe are not sufficient grounds for calling into question the parity assignments given by Martinez et al[2].

ACKNOWLEDGEMENT

The generous assistance of the USERDA through the Inorganic Materials Research Division of the Lawrence Berkeley Laboratory is gratefully acknowledged.

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2. G. Martinez, M. Schluter, and M. L. Cohen, Phys. Rev. B, 11, 651 (1975), Fig. 3.
3. B. Sapoval, J. de Physique 29, C4-133 (1968); Phys. Rev. B, 7, 5276 (1973).
4. W. W. Scanlon, SOLID STATE PHYSICS, F. Seitz and D. Turnbull, eds., (Academic Press, 1959), Volume 9, page 118.
5. See for example, L. I. Schiff, QUANTUM MECHANICS, Third Edition, (McGraw-Hill, 1968), pages 419-420.
6. One may estimate (see Reference 5) the relative intensities of allowed and forbidden electric dipole transitions for PbTe for the photon energy range in question. The forbidden transition would have a probability per unit time that is decreased by a factor $(ka)^2$ relative to that of the allowed transition. Here k is the magnitude of the wave vector of the incident radiation, and a is the spatial extent of the relevant wave function, in this case that of a valence band electron. Taking $\hbar\omega = 1.5$ eV as a typical value, $k = 0.76 \times 10^5$ cm^{-1}, and taking a approximately equal to a lattice constant (6.5×10^{-8} cm) gives $(ka)^2 = 2.4 \times 10^{-5}$. One would thus expect the intensity of a forbidden electric dipole transition to be about 10^{-5} of the intensity of an allowed transition. Typical values of $(\Delta R/R)$ for the PbTe spectra are not given in Glosser et al's Letter. However, from an earlier paper (R. Glosser et al, Phys. Rev. B, 1, 1607 (1969)) on electroreflectance studies of InSb, Fig. 2 suggests $(\Delta R/R) \approx 10^{-4}$ as a typical observed value, presumably for an allowed transition. An intensity 10^5 times smaller than this would be well below the minimum signal, $(\Delta R/R) \approx 10^{-7}$, quoted as detectable by Glosser. Further, an allowed but weak transition (e.g., a transition whose matrix

element is 100 times smaller than those observed) would also be below threshold since one would expect its intensity to be decreased by a factor of obout 10^4. The conclusion is that these electroreflectance spectra might be expected to exhibit a null result for both forbidden and allowed but weak electric dipole transitions. One would not then expect to tell the two apart experimentally on the basis of relative intensities.

7. S. Kohn, P. Y. Yu, Y. Petroff, Y. R. Shen, Y. Tsang, and M. L. Cohen, Phys. Rev. B, 8, 1477 (1973).

8. It should be noted that the L(4 → 6) transition in PbSe at 2.18 eV was characterized by the authors of Reference 7 as "weak". Therefore, this L(4 → 6) observation alone does not completely rule out L(4 → 6) being a forbidden electric dipole transition.

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