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Energy-Level Parities at L in PbTe

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The implications of the new parity labeling of the band states at L by Glosser, Kinoshita, and Rennex are discussed and shown to lead to properties which are difficult to reconcile with theoretical calculations and some experiments.

Glosser, Kinoshita, and Rennex[1] (GKR) have recently suggested that the accepted parities at the L point of the Brillouin zone for PbTe are inconsistent with their measurements of band-population effects in electroreflectance spectra. This is of particular interest since the minimum gap in this narrow-gap semiconductor is at L and the ordering of the states in this region is intimately related to the physical properties of this material.

The reordering of the levels involves bands 3 to 8 at L. There are five valence bands in PbTe and the gap (~0.2 eV) appears between bands 5 and 6, i.e., $L(6)-L(5)$. Most band-structure calculations on this material (and other Pb salts) yield positive parities for bands $L(3)$ to $L(5)$ and negative parities for bands $L(6)$ to $L(8)$. These include current-pseudopotential,[2,3] orthogonal-plane-wave,[4] augmented-plane-wave,[5] and Green's-function[6] calculations. The reordering suggested by GKR is based on nonobservation of critical-point transitions at L, and the subsequent conclusion that this implies that bands $L(5)$, $L(7)$, and $L(8)$ have one parity while bands $L(3)$, $L(4)$, and $L(6)$ have the other. GKR suggest that the above assignment would result in several parity-

TABLE I. Different proposed band orderings at the L gap of PbTe.

Band number	Standard ordering	GKR I ordering	GKR II ordering
$L(8)$	L_{45}^-	L_{45}^+	L_{45}^+
$L(7)$	L_6^-	L_6^+	L_6^-
$L(6)$	L_6^-	L_6^-	L_6^+
Gap	Gap	Gap	Gap
$L(5)$	L_6^+	L_6^+	L_6^-
$L(4)$	L_{45}^+	L_{45}^-	L_{45}^+
$L(3)$	L_6^+	L_6^-	L_6^+

forbidden transitions consistent with their observations. The GKR suggestion leads to two possible orderings (GKR I and GKR II) for the bands at L (given in Table I). We propose that both GKR I and GKR II orderings lead to properties of the electronic structure which are difficult to reconcile with theoretical calculations and some experiments.

Although GKR I and II are both in conflict with the calculated assignments, in the latter case the differences are only in the reversal of $L(5)$ and $L(6)$. Since this only requires a few tenths of an eV change, and since it may be argued that the results of band calculations are only accurate to about this range of energy, conclusions based on the calculated values for the energy levels at L are not sufficient to rule out GKR II at the outset (we will return to GKR II). However, in the case of GKR I the switching of four bands over a range of several eV is well within the domain of band-structure accuracy. In addition, charge-density calculations[7] indicate that bands 3 and 4 are approximately 80% p-like around Te. This is consistent with the atomic ordering of the Te and Pb p levels.[6] If the parity were changed, the increase of Pb p character over Te p character would be in conflict with the above.

Another consequence of GKR I involves the effective masses at the band gap. From $\vec{k}\cdot\vec{p}$ theory, the mass at the top of the valence band $L(5)$ has three negative contributions in the standard ordering coming from interactions of $L(5)$ with $L(6)$, $L(7)$, and $L(8)$. In GKR I, the interaction of $L(5)$ is with $L(6)$, $L(4)$, and $L(3)$. Because the latter two bands are lower in energy than $L(5)$, the sign of the interaction with $L(4)$ and $L(3)$ is reversed. This positive contribution tends to cancel the negative contribution from $L(6)$ and results in a larger band mass. Thus, the agreement[2] between theory and experiment is destroyed.

One theoretical argument which is in conflict with GKR II involves the pressure dependence of the $L(5)$ and $L(6)$ energy levels (the temperature dependence can also be used in a similar way). The pressure and temperature coefficients of the L_6^+ and L_6^- states have been computed and analyzed[7-11] in terms of wave-function symmetry. These calculations show that the gap decreases with pressure because s-like levels move up faster with pressure than p-like levels. Hence for PbTe the $L(5)=L_6^+$, $L(6)=L_6^-$ calculated pressure coefficient[8] for the gap is negative (-7.5×10^{-6} eV/bar) and in good agreement with experiment [$(-7.4\pm0.2)\times10^{-6}$ eV/bar]. If the GKR II ordering is adopted the calculations would give a positive pressure coefficient because of the symmetry[7] of the bands. This latter sign is found in most diamond and zinc-blende semiconductors and is explained[12] using the arguments above; the top of the valence band is usually p like while the bottom of the conduction band is usually s like.

A strong yet not completely conclusive experimental argument for an L_6^+ valence-band maximum is given by Knight-shift measurements.[13] These measurements suggest a strong s-like wave-function component around Pb for the top valence-band state which is inconsistent with GKR II.

It should also be mentioned that a change in the parity assignments for PbTe would result in changes for the other Pb salts,[14] Sn salts, and possibly Ge salts. This is because of the observation of band inversion or lack thereof in alloys of these materials with PbTe. In view of these consequences and the arguments presented here it would be helpful if new data could be made available to test the conclusions of GKR. Reflectivity and modulated reflectivity in the 0.8- to 2.2-eV range would be very helpful. Wavelength modulation, thermoreflectance, or piezoreflectance measurements would be particularly useful since some of the structure in GKR is weak (e.g., B') and critical-point location in electroreflectance data often depends on a detailed study of the line shape.[15]

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Equation (6) should read

$$ds^2 = \left(c_0 + \frac{f(r-t)}{r} + \frac{g(r+t)}{r}\right)^2 (-dt^2 + dr^2 + r^2\, d\Omega^2).$$

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Footnote 18, which reads "The calculated value ... is sensitive ... by 10 MeV," should read "The calculated value ... is insensitive ... by 10 MeV."