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Publication Date

1973-12-01

Submitted to Solid State Communications

LBL-2527
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December 1973

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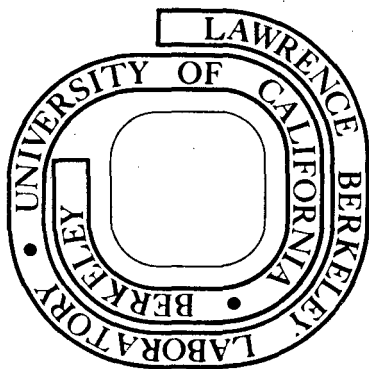
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Proposed Measurement of the Knight Shift in Lead Polonide (PbPo)

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ABSTRACT

It is suggested that a measurement of the Knight shift of ^{207}Pb in p-type lead polonide would provide information concerning the correctness of the inverted band structure recently proposed for PbPo.

In recent papers^{1,2}, it was proposed, based on empirical evidence, that the band structure of lead polonide (PbPo) may be inverted from the band structure of PbS, PbSe, and PbTe. In such an inverted band structure, the lowest conduction band in PbPo would be an L_6^+ state and the highest valence band an L_6^- state, leading to a negative value of the energy gap $E_0 \equiv E(L_6^-) - E(L_6^+)$ for PbPo. The calculated value¹ of E_0 for PbPo is approximately -0.1 eV at 80°K . A consequence of this inverted band structure is that the temperature coefficient of the energy gap for PbPo would be negative, in contrast to the well-known positive temperature coefficients observed in PbS, PbSe, and PbTe. The measurement of the sign of the temperature coefficient of the energy gap for PbPo thus offers an unequivocal test of the correctness of the proposed inverted band structure.

The object of this note is to suggest that a measurement of the Knight shift of ^{207}Pb in p-type PbPo should also provide information on the correctness of the proposed inverted band structure, and that this experiment might perhaps also be simpler in practice than a measurement of the sign of the temperature coefficient of the energy gap.

The band edge states in PbS, PbSe, and PbTe are such that the lowest conduction band is an L_6^- state and the highest valence band is an L_6^+ state, in

agreement with the Knight shift studies of Weinberg and Callaway³ on lead in p-type PbTe. Further, it appears that, from the work of Senturia et al⁴, the interaction between holes and lead nuclei in p-type PbTe can be described by a contact interaction⁵ between their magnetic moments. The conclusions of these workers concerning PbTe are as follows. The valence band edge state is s-like around the lead nuclei, i.e., it is an L_6^+ state (derived from an L_1 single group level). On the other hand, the L_6^- conduction band edge state (derived from an L_2 , single group level) is not s-like around the lead nuclei; this state can only produce smaller Knight shifts of orbital origin.

These facts suggest that a measurement of the Knight shift of ^{207}Pb in p-type PbPo would provide information on the character of its valence band edge. An inverted band structure for PbPo would mean a situation opposite to that described above for PbTe. If the valence band edge in PbPo is indeed an L_6^- state, then the wave function for this state would not be s-like around the lead nuclei. In such a case, the contact interaction between holes and ^{207}Pb nuclei in p-type PbPo would be expected to lead to a smaller Knight shift than is observed in p-type PbTe. This can be seen from the equation⁶

$$(\Delta H/H_0) \propto \langle |u_{\underline{k}}(0)|^2 \rangle_{E_F}, \quad (1)$$

where $(\Delta H/H_0)$ is the magnitude of the Knight shift in the applied magnetic field H_0 . The quantity $\langle |u_{\underline{k}}(0)|^2 \rangle_{E_F}$ is the square of the modulation part of the Bloch function $u_{\underline{k}}(\underline{r})\exp[j(\underline{k}\cdot\underline{r})]$ for holes, evaluated at the nucleus ($\underline{r} = 0$), and averaged over the Fermi surface at energy E_F . An L_6^- valence band edge would mean a lack of s-like character in the hole wave function about the lead nucleus, and the quantity $\langle |u_{\underline{k}}(0)|^2 \rangle_{E_F}$ would therefore be small. From equation (1), then, the magnitude of the Knight shift of ^{207}Pb in p-type PbPo would be expected to much smaller than its magnitude in p-type PbTe if the band structure of PbPo is indeed inverted from that of PbTe and the other lead salts.

In summary, a measurement of the magnitude of the Knight shift of ^{207}Pb in p-type PbPo would, on comparison with the magnitude of the shift in p-type PbTe, provide information on the correctness of the inverted band structure proposed for lead polonide.

ACKNOWLEDGEMENT

The author would like to thank the Department of Physics of the University of California at Berkeley for its kind hospitality while this work was being done. The generous assistance of the Inorganic Materials Research Division of the Lawrence Berkeley Laboratory is also acknowledged. Work done under the auspices of the U. S. Atomic Energy Commission.

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