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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 strructure, 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 $E_o \equiv E(L_6^-) - E(L_6^+)$ for PbPo. The calculated value[1] of E_o 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 <u>negative</u>, 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 Callaway[3] on lead in p-type PbTe. Further, it appears that, from the work of Senturia et al[4], the interaction between holes and lead nuclei in p-type PbTe can be described by a contact interaction[5] 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 <u>is</u> indeed an L_6^- state, then the wave function for this state would <u>not</u> 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 equation[6]

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

where $(\Delta H/H_o)$ is the magnitude of the Knight shift in the applied magnetic field H_o. 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 <u>if</u> 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.

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