and leads to large oscillations in Reσ.

For helicon waves propagating in metals $\hbar\omega \ll kT$ and Eq. (4) becomes

$$\mathrm{Re}\sigma(Q)=\frac{3\pi Ne^2}{4mQv_F}\left[1-\left(\frac{\omega_c-\omega}{Qv_F}\right)^2\right]\frac{\hbar\omega_c}{kT}$$

$$\times\cosh^{-2}\left[\frac{E_F-(n_0+\frac{1}{2})\hbar\omega_c-\hbar^2k_{z0}{}^2/2m}{2kT}\right] \tag{6}$$

where n_0 is the integer for which the argument of the cosh function is a minimum. The relation (6) describes oscillations of giant amplitude $(\sigma_R^{\mathrm{Max}}-\sigma_R^{\mathrm{Min}})\gg\sigma_R^{\mathrm{Min}}$ in the real part of the conductivity which are approximately periodic in H^{-1} with a period given by

$$\Delta\left(\frac{1}{H}\right)=\frac{e\hbar}{mE_Fc}\,\frac{1}{1-[(\omega_c-\omega)/Qv_F]^2}. \tag{7}$$

The attenuation coefficient Q_I is found from (2) to be proportional to $[(\sigma_I{}^2+\sigma_R{}^2)^{1/2}-\sigma_I]$ in the qualitative sense previously discussed and hence also shows giant oscillations with the period (7). The denominator in (7) is a slowly varying function of H compared to the very short de Haas–van Alphen period in metals. No giant oscillations occur in Im$\sigma(Q)$ since the summation over k_z is not restricted. Thus the real part of Q, Q_R, is given by the usual helicon dispersion relation $Q_R\simeq(4\pi Ne\omega/cH)^{1/2}$. The onset of the absorption is at $Qv_F=\omega_c-\omega$.[2-4]

When we consider Alfvén waves in semimetals, we need to evaluate (4) in the limit $\hbar\omega\gg kT$ and sum over both electrons and holes. The initial state taking part in the transition can now be in a band of energies from E_F to $E_F-h\omega$ with a fixed k_z value given by (5) for electrons and for holes. The number of Landau levels contributing to the attenuation will therefore oscillate. It has been shown[6,7] that attenuation occurs below a threshold value defined as the field where the equality $\omega_c=\omega+v_FQ_R$ is satisfied for any carrier. The real part of the wave number is given by $Q_R=\omega H^{-1}\times(4\pi\sum N_jm_j)^{1/2}$ and the sum is over all carriers.[5] Below the onset the attenuation will thus be oscillatory with each carrier contributing with a period given by Eq. (7).

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RELATIVISTIC EFFECTS IN THE BAND STRUCTURE OF PbTe*

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The purpose of this Letter is to point out that relativistic interactions have a drastic effect on the energy band structrue of PbTe and are of major importance in understanding the energy gaps and effective masses. These interactions are commonly derived by converting the 4-component Dirac equation into a second-order equation and then reducing this to a two-component form. When this is done, as in the Pauli approximation, two other terms appear besides the spin-orbit interaction, namely, the mass-velocity energy correction and a term of the form $(i\mu_0/2mc)\vec{\epsilon}\cdot\vec{p}$, where $\vec{\epsilon}$ is the electric field seen by an electron and $\vec{p}$ is its momentum. If the spatial components of the vector potential are assumed to be zero, the one-electron Hamiltonian is[1]

$$\mathcal{H}=-(\hbar^2/2m)\nabla^2-e\varphi-(1/2mc^2)(E+e\varphi)^2$$
$$-(i\mu_0/2mc)\vec{\epsilon}\cdot\vec{p}+(\mu_0/2mc)\vec{\sigma}\cdot(\vec{\epsilon}\times\vec{p}).$$

We show in this Letter that the mass-velocity term $(-1/2mc^2)(E+e\varphi)^2$ and the term $-(i\mu_0/2mc)\times\vec{\epsilon}\cdot\vec{p}$ have a very marked effect on the (111) band edge of PbTe.

The mass-velocity and $\vec{\epsilon}\cdot\vec{p}$ terms will be largest when an electron is near the nucleus. Since the atomic orbitals behave as r^l for small r, s functions will have the largest energy shifts. Even in the hydrogen atom these corrections to the $2s$ energy are several times larger than the spin-orbit splitting of the $2p$ level. In a solid the one-electron wave functions do not have a definite orbital angular momentum and it is common for a Bloch function to start at the center of the Brillouin zone predominately of one l character and at a zone edge to have a different l character. That is, regarded as a function of k, the Bloch function associated with a particular band has a different admixture of $s, p, d, \cdots$ character at different points of the zone. Thus if the Bloch function were p-like at $k=0$ and s-like at an edge, these relativistic corrections could substantially change the band shape at the edge but only slightly at the center. Therefore, these corrections are k dependent and will affect both energy gaps and effective masses.

This reasoning has led us to include the mass-velocity and $\vec{\epsilon}\cdot\vec{p}$ terms in an augmented plane-wave (APW) investigation of the band structure of PbTe. The results obtained so far are so striking that we feel they should be presented here in advance of a full discussion. We wish to stress that it is the relativistic effects that we are concerned with here and for that reason we leave aside the quantitative nature of the bands. In brief, the APW scheme has been carried out for PbTe for several ionicities and the results given here are for zero ionicity. The bands were first found using a crystal potential constructed from atomic potentials for the Pb and Te atoms kindly supplied by Herman. These "unperturbed" band energies are given in the left-hand column of Fig. 1 at the (111) zone edge where experiment indicates the top of the valence band and bottom of the conduction band to be.

The valence-conduction band gap for the "unperturbed" bands is between L_2' and L_3' and is seen to be about 1.51 eV. The effect of the spin-orbit interaction was taken into account not by first-order perturbation theory but by setting up the 12×12 secular equation arising from the L_3, L_2', L_3', and L_1 bands and finding the eigenstates and energies. These energies are shown in the middle column of Fig. 1. The spin-orbit splitting of the "unperturbed" bands is apparent and now the gap occurs between the two L_6^- states and is 1.37 eV.

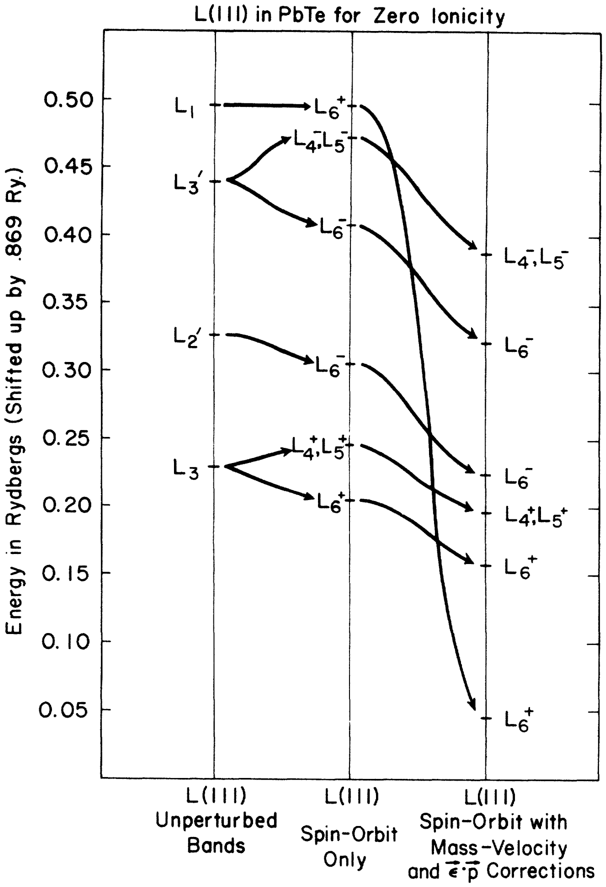

FIG. 1. Results at the (111) zone edge for PbTe with zero ionicity.

Regarding these spin-orbit states as a new basis set, the 12×12 energy matrix due to the mass-velocity and $\vec{\epsilon}\cdot\vec{p}$ corrections was set up and the corresponding secular equation solved resulting in the energies shown in the right-hand column of Fig. 1. The drastic change in the band energies is evident. The upper L_6^+ in the middle column is s-like about the Pb and will experience the greatest relativistic shift since these effects are a rapidly increasing function of atomic number. This is indeed the case as shown in Fig. 1 where the L_6^+ state shifts from the highest to the lowest lying level. Away from L the L_6 bands become Λ_6 and cannot cross so that this depression of the L_6^+ state does not make PbTe a metal. Now the gap lies between the L_4^+, L_5^+ level and the L_6^- level and it has dropped from 1.37 eV to 0.40 eV in much closer agreement with experiment which indicates a value of about 0.3 eV. Furthermore, the lowest three bands belonging to the valence set all have even parity while the three upper bands all have odd parity. Therefore, an optical transition would be allowed at *L* across the gap and this also satisfies the conditions required by the $\vec{k}\cdot\vec{p}$ perturbation method for small effective masses both for holes and electrons at *L*. This agreement with experiment is seen to be entirely due to including these relativistic corrections.

It is interesting to compare these results obtained for the solid with the relativistic shifts for the isolated Pb and Te atoms which have been found by Herman and Skillman.[2] They are shown in Fig. 2. A tight-binding analysis of the PbTe case shows that at *L* the *p* functions of Pb do mix with the *s* functions of Te but not with the Te *p* orbitals. However, at $k=0$ symmetry forbids *s*-*p* mixing. Any *s*-*p* mixing will be very important at *L* because of the much larger corrections to the *s* energies. Let us assume, however, that the conduction band at *L* is given only in terms of the 6*p* functions of Pb and the valence band only in terms of the 5*p* functions of Te. Then the atomic results shown in Fig. 2 would indicate a decrease in the energy gap at *L* of 0.42 eV since the relativistic effects depress the Pb-6*p* energy more than the Te-5*p* energy. This very qualitative argument shows that the free atom results indicate the presence of the gap change for the solid. The much larger gap change obtained in the APW calculation is presumably due to *s*-*p* mixing. The relativistic effects evaluated in this paper and the free atom relativistic results of reference 2 have not been found by including these interactions in a self-consistent field calculation. However, Waber[3] has done this for the free Pb and Te atoms by self-consistently solving the Dirac equation. His results are very close to those of Herman and Skillman indicating that self-consistent corrections are not of great importance.

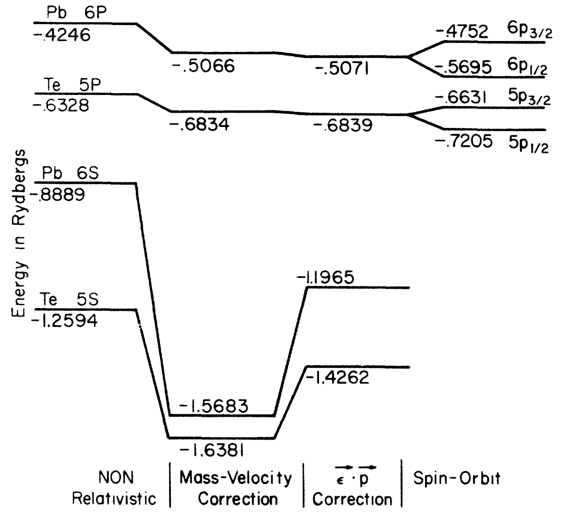

FIG. 2. The energy levels of the atomic 5*s* and 5*p* functions of Te and 6*s* and 6*p* levels of Pb as taken from the work of Herman and Skillman, reference 2.

It is quite clear from these results that the mass-velocity and $\vec{\epsilon}\cdot\vec{p}$ terms will be absolutely essential in many band calculations and will lead to major corrections. Without them the band energies and effective masses at the point *L* in PbTe would be meaningless. Furthermore, it can be expected that these terms will lead to substantial shifts in *s*-like impurity levels as already indicated by Appel.[4]

The authors wish to thank the staff of Massachusetts Institute of Technology Cooperative Computing Laboratory for their cooperation in the preparation of these numerical results.

After this Letter was submitted, it came to our attention that Herman, Kuglin, Cuff, and Kortum have been considering independently the problem of relativistic effects on energy band structures and were submitting a Letter[5] discussing their treatment.

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