COMMENTS AND ADDENDA

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Effect of $p_{3/2}$ Intraband Polarization on the Mobility of Zero-Gap Semiconductors*

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It is shown that in doped zero-gap semiconductors like α-Sn, the intraband part of the static screening function is considerably decreased from that of free electrons at large momentum transfer by the p-like character of the conduction-band wave function. However, it is also shown that this large screening loss produces a relatively small change in the ionized-impurity-limited mobility.

Recently, there has been considerable interest in the dielectric function and low-temperature electron mobility of symmetry-induced zero-gap semiconductors.[1-12] Liu and Brust[1,2] showed that, in the degenerate limit, the random-phase approximation[13-15] (RPA) interband dielectric function diverges like q^{-1} as $q \to 0$ in an intrinsic material of this kind. Liu and Tosatti[4,5] showed that impurity carriers remove this singularity leaving a finite dielectric constant which is strongly dependent on impurity concentration and greatly enhanced over the background dielectric constant. Broerman[9] examined the dielectric function at nonzero temperature and showed that thermally excited carriers also remove the singularity leaving a dielectric constant which is strongly temperature and impurity-concentration dependent.

Liu and Tosatti[4,5] showed that the low-concentration enhancement of the dielectric constant produces an enhancement of the ionized-impurity-limited mobility which is in good agreement with that observed[16,17] at liquid-He temperatures in n-type samples of α-Sn. However, Broerman[3] showed that a mobility enhancement is also produced by the reduction in large angle scattering cross sections arising from the $p_{3/2}$-like character of the conduction-band wave function. He then showed that when both the RPA-dielectric-function enhancement and the reduction in large angle scattering are taken into account, the calculated[7] mobilities are about three times larger than experiment,[16,17] while a calculation[6] with the background dielectric constant alone yields values in good agreement with experiment. On the other hand, a calculation[8] including both the RPA dielectric function and the $p_{3/2}$ scattering matrix element is in good agreement with experiment in HgSe[18,19] and HgTe.[20] Broerman[10] has suggested, on the basis of the anomalous shape observed by Lavine and Ewald[21] of the mobility enhancement produced by L_6^+-electron screening above a donor concentration of 5×10^{17} cm^{-3}, that the anomalously low mobility of α-Sn is due to additional scattering on neutral defects in the available samples.

None of the above calculations has considered the modifications produced in the intraband part of the RPA dielectric function ("free-electron" screening) by the $p_{3/2}$ character of the conduction-band wave function. In this paper we will show that the angular dependence of the conduction-band overlap matrix element produces a large decrease in the high-momentum-transfer intraband screening. However, we will also show that this large screening loss produces only a small decrease in the ionized-

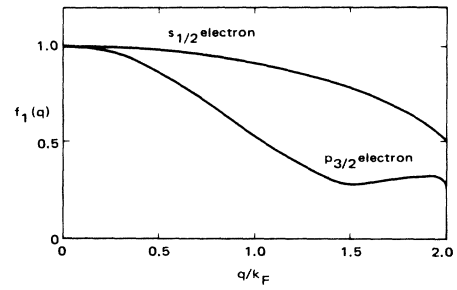

FIG. 1. The intraband screening functions for $s_{1/2}$ electrons (upper curve) and $p_{3/2}$ electrons (lower curve).

impurity-limited mobility.

The dielectric function is conveniently separated into an interband part $4\pi\alpha^{\text{inter}}$ arising from the Γ_8 bands near $k=0$, a background interband part ϵ_0 due to all other bands, and an intraband part $4\pi\alpha^{\text{intra}}$:

$$\epsilon(q)=\epsilon_0+4\pi\alpha^{\text{inter}}+4\pi\alpha^{\text{intra}}. \tag{1}$$

Liu and Tosatti[4,5] have calculated $4\pi\alpha^{\text{inter}}$ for a parabolic band in the degenerate limit. They obtain

$$4\pi\alpha^{\text{inter}}=(8e^2\mu m_0/\pi\hbar^2 k_F)[1-a'(q/k_F)^2], \tag{2}$$

where k_F is the Fermi momentum and $a'\sim\frac{1}{12}$. Broerman[7] has shown that this is a good approximation for the nonparabolic conduction band of the Kane[22] model. The RPA intraband polarization can be similarly calculated according to

$$4\pi\alpha^{\text{intra}}(q)=\frac{8\pi e^2}{q^2}\sum_{k<k_F}\frac{|(u_{\vec{k}},u_{\vec{k}+\vec{q}})|^2}{E_{\vec{k}+\vec{q}}-E_{\vec{k}}}(1-f_{\vec{k}+\vec{q}}), \tag{3}$$

where $u_{\vec{k}}$ is the periodic part of the conduction-band wave function. The matrix element $|(u_{\vec{k}},u_{\vec{k}+\vec{q}})|^2$ can be calculated in the Kane three-band approximation ($\vec{k}\cdot\vec{p}$ interaction of Γ_8^+, Γ_7^+, and Γ_7^-) to be

$$|(u_{\vec{k}},u_{\vec{k}+\vec{q}})|^2=\sum_{n=0}^{2}\rho_n(\xi_k,\xi_{|\vec{k}+\vec{q}|})x^n, \tag{4}$$

where

$$x=\vec{k}\cdot(\vec{k}+\vec{q})/|\vec{k}||\vec{k}+\vec{q}|, \tag{5}$$

$$\rho_0=(aa_+)^2+\tfrac{1}{4}(bb_+)^2-bb_+\frac{bc_++cb_+}{\sqrt{2}}+\frac{(bc_++cb_+)^2}{2}, \tag{6}$$

$$\rho_1=2(aa_+)(bb_++cc_+), \tag{7}$$

$$\rho_2=\tfrac{3}{4}(bb_+)^2+bb_+\frac{(bc_++cb_+)}{\sqrt{2}}+2(bb_+)(cc_+)-\tfrac{1}{2}(bc_++cb_+)^2+(cc_+)^2. \tag{8}$$

Here a, b, and c are, respectively, defined by Eqs. (10)–(12) of Ref. 7, $\xi_k=E_k/E_g$ where E_g is the $\Gamma_8^+-\Gamma_7^-$ splitting, and the subscript $(+)$ denotes evaluation of the quantity at $\xi_{|\vec{k}+\vec{q}|}$. In the parabolic limit, which corresponds to $\xi_k\to 0$, $\xi_{|\vec{k}+\vec{q}|}\to 0$, Eq. (4) reduces to

$$|(u_{\vec{k}},u_{\vec{k}+\vec{q}})|^2=\tfrac{1}{4}(1+3x^2). \tag{9}$$

Evaluation of $4\pi\alpha^{\text{intra}}$ using the nonparabolic matrix element of Eq. (4) proves to be excessively cumbersome. The parabolic approximation of Eq. (9) is essentially exact for carrier concentrations below 5×10^{16} cm^{-3} and in this approximation $4\pi\alpha^{\text{intra}}$ is given by

$$4\pi\alpha^{\text{intra}}=(k_{\text{FT}}^2/q^2)f_1(q), \tag{10}$$

where k_{FT} is the Fermi-Thomas momentum, and $f_1(q)$ is shown in Fig. 1. As can be seen, the screening at large momentum transfer is greatly reduced from that of a free[23] (or $s^{1/2}$) electron.

In performing the scattering calculation, we make the following approximations. We approximate $f_1(q)$ by

$$f_1(q)=1-a''(q/k_F)^2+a'''(q/k_F)^4, \tag{11}$$

with $a''=0.47$ and $a'''=0.075$. This approximation has a slightly positive slope at $q=2k_F$, while $f_1(q)$ actually has a negative infinite slope at this point, arising from a logarithmic singularity in the derivative of $f_1(q)$. Over most of the range of q, the approximation slightly underestimates $f_1(q)$. In order to partially account for nonparabolic effects, we use the expression (19) of Ref. 7 (without the Friedel correction, which is negligible) for k_{FT}^2. It should be noted that these approximations yield exact values for $q^2 4\pi\alpha^{\text{intra}}$ in the limit $q\to 0$ at all concentrations. As will be seen, the mobility is quite insensitive to the values of the high-momentum-transfer screening, especially at high-impurity concentrations where the approximations in the q dependence of $4\pi\alpha^{\text{intra}}$ are worst. Thus we feel that, for the purposes of a mobility calculation, these approximations are quite good. Since the main omission from the calculation of $f_1(q)$ is now the $s_{1/2}$ part of the wave function, whose matrix element has no angular dependence and thus produces less q dependence in $4\pi\alpha^{\text{intra}}$, the net result should be a slight underestimate of the screening and hence of the mobility. The only changes necessary in the theory of Ref. 7 to accommodate the $p_{3/2}$ intraband polarization effect are the following redefinitions of the constants A, B, and C [Eqs. (16)–(18), respectively] appearing in the scattering integral Φ:

$$A=2\left(\frac{k}{k_F}\right)^2\left[a'''\frac{k_{\text{FT}}^2}{k_F^2\epsilon_I(0)}-\left(1-\frac{\epsilon_0}{\epsilon_I(0)}\right)a'\right], \tag{12}$$

$$B=-1+\frac{k_{\text{FT}}^2}{k_F^2\epsilon_I(0)}\left[a''-4a'''\left(\frac{k}{k_F}\right)^2\right]+4\left(\frac{k}{k_F}\right)^2\left(1-\frac{\epsilon_0}{\epsilon_I(0)}\right)a', \tag{13}$$

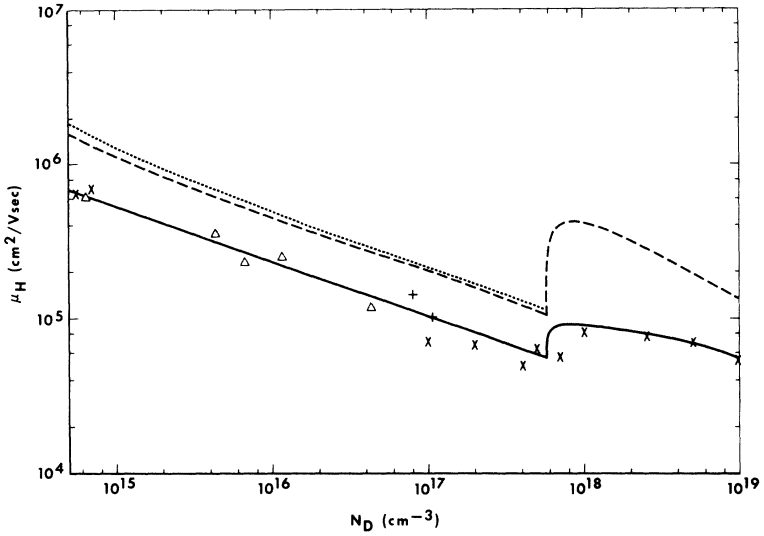

FIG. 2. Ionized-impurity-limited mobility of degenerate n-type α-Sn. The dotted curve is the calculation of Ref. 7, using $p_{3/2}$ RPA interband polarization and a q-independent free-electron intraband polarization. The dashed curve is a calculation using $p_{3/2}$ RPA interband and intraband polarization. The solid curve is the dashed curve superimposed on a neutral scattering mechanism with an electron-concentration-independent mean free path of 1.95×10^{-4} cm. The experimental points are from Ref. 21 (×), Ref. 17 (△) and Ref. 16 (+).

$$C=\frac{1}{2k^2}\left\{\frac{k_{FT}^2}{\epsilon_I(0)}\left[1-2a''\left(\frac{k}{k_F}\right)^2+4a'''\left(\frac{k}{k_F}\right)^4\right]\right.$$

$$\left.+2k^2\left[1-2\left(\frac{k}{k_F}\right)^2\left(1-\frac{\epsilon_0}{\epsilon_I(0)}\right)a'\right]\right\}\ . \quad (14)$$

The result of this calculation for α-Sn is the dashed curve of Fig. 2. The dotted curve is the calculation of Ref. 7, which used RPA interband polarization and q-independent Fermi-Thomas screening for the intraband polarization. The abscissa is donor concentration, which is the same as electron concentration up to 5×10^{17} cm^{-3}. Above this we have included screening by the L_6^+ electrons[21,10] whose band edge lies at 0.092 eV. The reduction in $p_{3/2}$ screening produces a lowering of mobility ranging from about 15% at the lowest concentrations to about 5% at 5×10^{17} cm^{-3}. Thus, it is quite a small effect. One can understand this result qualitatively by noting that $4\pi\alpha^{\text{intra}}$ appears in the calculation in the form $[k_{FT}^2 f_1(q)+q^2\epsilon_I(q)]^{-2}$, where $\epsilon_I(q)=\epsilon_0+4\pi\alpha^{\text{inter}}$. At high momentum transfers, which are heavily weighted by the Boltzmann equation and where most of the screening losses occur, k_{FT}^2 is relatively less important than $q^2\epsilon_I(q)$. The effect on the mobility should decrease with increasing concentration since k_{FT}^2 grows less rapidly than $k_F^2\epsilon_I$ $(2k_F)$. The solid curve in Fig. 2 is a superposition of RPA screened ionized-impurity scattering (dashed curve) on a scattering process[10] with an electron-concentration-independent mean free path of 1.95×10^{-4} cm. It is in excellent agreement with the data.

Finally, a comment on the other two symmetry-induced zero-gap structures[8] HgSe and HgTe. For HgSe there is essentially no change in the conclusion of Ref. 8 since all the data lie above 2×10^{17} cm^{-3}. For HgTe, the theory now lies about 12% lower than the value for the highest-mobility sample of Ivanov-Omskii *et al.*[20] Since the experimental uncertainty may be this large, the disagreement may have no significance. On the other hand, it may be that this is a manifestation of the effect of the valence-band overlap, caused by the linear terms in the Λ_4, Λ_5 parts of Γ_8, on the interband polarization.

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Diffusion in Transient Space-Charge-Limited Currents*

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The recent analysis by Batra, Schechtman, and Seki neglects charge-carrier diffusion in transient space-charge-limited currents (SCLC) in photoconductor-dielectric structures. It is pointed out that such an analysis cannot predict the initial diffusion-dominated current observed by high-resolution experimental measurements. Recent work which develops the necessary mathematical theory for determining transient SCLC with diffusion is cited.

The preliminary theory for time-dependent space-charge-limited currents (SCLC) with charge-carrier diffusion *neglected* was presented by Many and Rakavy[1] and has been applied recently to photoconductor-dielectric structures by Batra, Schechtman, and Seki.[2] A more complete theory of transient SCLC with charge-carrier diffusion *included* has been developed by the present author.[3] It was shown in the latter work that diffusion effects dominate the current density during the initial stage of transient SCLC with an $E=0$ boundary condition and cannot be neglected if one desires to predict or interpret high-resolution experimental measurements[4] in a quantitative fashion. Since an $E=0$ boundary condition is featured at the photoconductor-dielectric interface (where the drift-current density vanishes and the diffusion-current density regulates the local charge-carrier flow) in the model considered by Batra, Schechtman, and Seki, diffusion effects must be taken into account in solving for the transient SCLC in photoconductor-dielectric structures that feature a characteristic diffusion time[3] $t_1 \equiv 4DL^2/\mu^2V^2$ which is large compared to the rise time of the light pulse. Such would ordinarily be the case for the photoconductor-dielectrics at field strengths V/L less than about 100 V/cm. The mathematical theory needed for solving the photoconductor-dielectric and other related transient-diffusion SCLC problems has been advanced recently in a detailed and comprehensive work by Eckstut.[5]

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