a result of the small magnitude of the uniaxial deformation potential constant Σ_μ. The reason for the small value of Σ_μ can be understood, at least qualitatively, on the basis of the energy band-structure calculations of Kahn and Leyendecker.[1] If the Ti-Ti overlap is neglected, the lowest-lying conduction band ($\Delta_{2'}$) is flat along the cubic axes because the $\Delta_{2'}$ titanium 3d orbital does not mix with any of the oxygen $2p$ orbitals. The main effect of an elastic strain along a cubic axis is to change the Ti-O separation, but this will not cause any shift in the energy of the $\Delta_{2'}$ band. Therefore, the deformation potential, which defines the change in energy of the $\Delta_{2'}$ band at the X point with strain, is zero. The inclusion of the Ti-Ti overlap causes the lowest lying $\Delta_{2'}$ conduction band to curve downward slightly along the cubic axes[1] and this leads to a small deformation potential that is qualitatively in agreement with the experimental piezoresistance results.[6]

In summary, we have measured the weak-field magnetoresistance coefficients in Nb-doped $SrTiO_3$ at 4.2, 77, and 120°K. The magnetoresistance results at 77 and 120°K are consistent with a band structure consisting of minima along the ⟨100⟩ reciprocal axes. The phase transition at 110°K does not have a significant effect on the magnetoresistance results. We postulate that the absence of a large piezoresistance effect in cubic $SrTiO_3$ due to the electron-transfer mechanism is a result of the small magnitude of the uniaxial deformation potential constant.

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Dielectric Singularity of α-Sn*

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The wave-number-dependent dielectric function $\epsilon(q)$ for the zero-gap semiconductor α-Sn has been calculated in the limit $q \rightarrow 0$. Because of the specific symmetry of the wave functions at the point of contact between the conduction and valence bands, $\epsilon(q)$ has a singularity of the form of $1/q$ in the long-wavelength limit. The screening of an impurity charge by this singular dielectric function is also discussed.

I. INTRODUCTION

THE response of a many-electron system to an external perturbation can be discussed most generally in terms of a frequency- and wave-number-dependent dielectric constant $\epsilon(\mathbf{q},\omega)$.[1,2] This is a very important quantity because it contains a great deal of information about the properties of the electron system in addition to the system's response to external probes. However, the actual evaluation of $\epsilon(\mathbf{q},\omega)$ even in the framework of random-phase approximation is generally very difficult if the system under consideration is other than a free-electron gas. Under certain circumstances, when only the effect of a static perturbation ($\omega=0$) is needed, the task becomes considerably simpler. For example, the static dielectric constant $\epsilon(\mathbf{q})$ for a semiconductor has been calculated in a spherically symmetric model band structure with one parameter representing an average energy gap.[3]

The purpose of this paper is to calculate $\epsilon(\mathbf{q})$ near $\mathbf{q}=0$ for the semiconductor α-Sn based on the zero-gap band model.[4] As we shall subsequently demonstrate, the dielectric function $\epsilon(\mathbf{q}) \propto 1/q$ as $q \rightarrow 0$. This behavior is a direct consequence of the nonaccidental nature of the valence-conduction-band contact at the zone center. Therefore, in terms of the existence of a long-wavelength singularity in the static dielectric constant, the dielectric response of α-Sn is between that of a conventional semiconductor [$\epsilon(\mathbf{q}) \rightarrow$ const as $q \rightarrow 0$] and that of a simple metal [$\epsilon(\mathbf{q}) \propto 1/q^2$ as $q \rightarrow 0$].

In view of the existence of a new type of singularity in the dielectric constant, we also discuss here its effects on the formation of impurity states and in the carrier mobility when the dominating scattering mechanism is due to ionized impurities.

II. CALCULATION OF MATRIX ELEMENT

The expression for $\epsilon(\mathbf{q})$ for a real solid in the framework of random-phase approximation has been ob-

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[1] J. Lindhard, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. **28**, 8 (1954).

[2] P. Nozières and D. Pines, Nuovo Cimento **9**, 470 (1958); Phys. Rev. **109**, 762 (1958).

[3] D. Penn, Phys. Rev. **128**, 2093 (1962).

[4] S. Groves and W. Paul, Phys. Rev. Letters **11**, 194 (1963).

tained by several authors[2,5] as

$$\epsilon(\mathbf{q})=1-\frac{4\pi e^2}{q^2}\sum_{n,n',\mathbf{k}}|\langle\mathbf{k},n|e^{-i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k}+\mathbf{q},n'\rangle|^2 \times\frac{N_{\mathbf{k}+\mathbf{q},n'}-N_{\mathbf{k},n}}{E_{\mathbf{k}+\mathbf{q},n'}-E_{\mathbf{k},n}},\quad(2.1)$$

where the matrix element $\langle\mathbf{k},n|e^{-i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k}+\mathbf{q},n'\rangle$ involves the Bloch wave function $|\mathbf{k},n\rangle$ with band index n and reduced wave vector $\mathbf{k}$, which is an eigenfunction of the one-particle Hamiltonian for an electron in the unperturbed periodic lattice with a corresponding energy eigenvalue $E_{\mathbf{k},n}$. The occupation number for the state $|\mathbf{k},n\rangle$ is denoted by $N_{\mathbf{k},n}$.

We first evaluate the matrix element in (2.1), which is just the overlap integral between the spatially periodic part of the two Bloch functions involved. We evaluate this part of the wave function by using the $\mathbf{k}\cdot\mathbf{p}$ perturbation method.

In α-Sn the conduction and valence bands make contact at the zone center and the degenerate band edge has Γ_8^+ symmetry. Therefore the structure of the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian in the vicinity of this degenerate state is the same as that for the valence-band edge of Ge or Si. It is well known that the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian H associated with this band edge can be represented by a 4×4 matrix for sufficiently small values of k.[6] The form of this matrix is given by several authors,[7] which we reproduce in the following:

$$H=\begin{bmatrix}\frac{1}{2}P & 0 & R & S\\ 0 & \frac{1}{2}P & -S^* & R^*\\ R^* & -S & \frac{1}{6}P+\frac{2}{3}Q & 0\\ S^* & R & 0 & \frac{1}{6}P+\frac{2}{3}Q\end{bmatrix},\quad(2.2)$$

where

$$P=2Ak^2+B(k_x^2+k_y^2-2k_z^2),$$
$$Q=Ak^2-B(k_x^2+k_y^2-2k_z^2),$$
$$R=-(N/\sqrt{3})(k_x-ik_y)k_z,$$
$$S=-(1/2\sqrt{3})[3B(k_x^2-k_y^2)-2iNk_xk_y].$$

The symmetry of the state under consideration requires the use of three constants A, B, and N in the matrix.

We find it convenient to write H in (2.2) in terms of the Dirac γ matrices in the following explicit representation:

$$\gamma^0=\begin{pmatrix}I & 0\\ 0 & -I\end{pmatrix},$$

$$\gamma^\alpha=\begin{pmatrix}0 & \sigma_\alpha\\ -\sigma_\alpha & 0\end{pmatrix},\quad(\alpha=1,2,3)$$

$$\gamma_5=\gamma^0\gamma^1\gamma^2\gamma^3=-i\begin{pmatrix}0 & I\\ I & 0\end{pmatrix},$$

where I is a 2×2 unit matrix and the three σ_α's are the Pauli spin matrices, σ_3 being diagonal. Using these γ matrices, we can rewrite (2.2) as

$$H=Ak^2+\tfrac{1}{2}B[(k_x^2+k_y^2-2k_z^2)\gamma^0-\sqrt{3}i(k_x^2-k_y^2)\gamma^2] +i(N/\sqrt{3})(k_xk_y\gamma^1+k_yk_z\gamma^3-k_zk_x\gamma_5).\quad(2.3)$$

The eigenvalues of H can be obtained easily as

$$E^\pm(\mathbf{k})=Ak^2 \pm[B^2k^4-C^2(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)]^{1/2},\quad(2.4)$$

each being doubly degenerate as required by Kramer's theorem. The constant C^2 is related to B and N as follows:

$$C^2=3B^2-\tfrac{1}{3}N^2,$$

and its magnitude determines the degree of warping of the surfaces of constant energy. Corresponding to each energy eigenvalue $E^+(k)$ or $E^-(k)$ in (2.4), we have two linearly independent eigenfunctions expressed by "spinor" functions as

$$\psi^\pm=\begin{pmatrix}u_1^\pm\\ u_2^\pm\end{pmatrix},$$

where both u_1 and u_2 are two-component "spinors." Using the Hamiltonian H in (2.3), we can immediately write down two coupled equations for u_1 and u_2 as follows:

$$[Ak^2+\tfrac{1}{2}B(k_x^2+k_y^2-2k_z^2)]u_1^\pm+i[-\tfrac{1}{2}\sqrt{3}B(k_x^2-k_y^2)\sigma_2 +(N/\sqrt{3})(k_xk_y\sigma_1+k_yk_z\sigma_3+ik_zk_x)]u_2^\pm =E^\pm(k)u_1^\pm,\quad(2.5)$$

$$[Ak^2-\tfrac{1}{2}B(k_x^2+k_y^2-2k_z^2)]u_2^\pm+i[\tfrac{1}{2}\sqrt{3}B(k_x^2-k_y^2)\sigma_2 -(N/\sqrt{3})(k_xk_y\sigma_1+k_yk_z\sigma_3-ik_zk_x)]u_1^\pm =E^\pm(k)u_2^\pm.$$

From the structure of the coupled equations in the above it is evident that for each of the energy eigenvalue $E^+(k)$ or $E^-(k)$ there are two linearly independent eigenvectors and they can be expressed in the following

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[5] H. Ehrenreich and M. H. Cohen, Phys. Rev. **115**, 786 (1959).

[6] For the valence-band edge in Si or Ge, this means that $E(\mathbf{k})-E(0)$ should be small compared with the spin-orbit splitting. For α-Sn, however, the energy difference $E(\Gamma_8^+)-E(\Gamma_7^-)$ is smaller than the spin-orbit splitting and it replaces the latter as the criterion for determining the region of k in which the 4×4 $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian is approximately valid.

[7] G. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev. **98**, 368 (1955); E. O. Kane, J. Phys. Chem. Solids **1**, 82 (1956). The relative phases of the basis functions are chosen differently in these two papers. We follow here Kane's choices. However, the ordering of the basis functions in setting up the matrix is different from either of the two papers.

way (except for a normalization factor):

$$E^+(k):\quad \psi_1{}^+\approx\begin{bmatrix}1\\0\\ \Lambda^+\begin{pmatrix}1\\0\end{pmatrix}\end{bmatrix},\quad \psi_2{}^+\approx\begin{bmatrix}0\\1\\ \Lambda^+\begin{pmatrix}0\\1\end{pmatrix}\end{bmatrix};$$

$$E^-(k):\quad \psi_1{}^-\approx\begin{bmatrix}\Lambda^-\begin{pmatrix}1\\0\end{pmatrix}\\1\\0\end{bmatrix},\quad \psi_2{}^-\approx\begin{bmatrix}\Lambda^-\begin{pmatrix}0\\1\end{pmatrix}\\0\\1\end{bmatrix}. \tag{2.6}$$

The operators $\Lambda^\pm$ can be obtained from Eq. (2.5) as

$$\begin{aligned}\Lambda^\pm=i[E^\pm(\mathbf{k})-Ak^2\pm\tfrac{1}{2}B(k_x{}^2+k_y{}^2-2k_z{}^2)]^{-1}&\\ \times[\pm\tfrac{1}{2}\sqrt{3}B(k_x{}^2-k_y{}^2)\sigma_2&\\ \mp(N/\sqrt{3})(k_xk_y\sigma_1+k_yk_z\sigma_3\mp ik_zk_x)].&\end{aligned} \tag{2.7}$$

Using (2.6) and (2.7), it is a straightforward matter to obtain the normalized eigenfunctions for the two energy eigenvalues involved. However, we choose to write them down explicitly only for the special case where the constant C in (2.4) is equal to zero (or $N=\pm 3B$).[8] Expressed in terms of the spherical coordinates (k,θ,ϕ) of the wave vector $\mathbf{k}$, they are given by the following:

$$E^+(\mathbf{k})=(A+B)k^2:$$

$$\psi_1{}^+=\begin{bmatrix}\frac{1}{2}\sqrt{3}\sin\theta\\0\\-\cos\theta\, e^{i\phi}\\-\frac{1}{2}\sin\theta\, e^{2i\phi}\end{bmatrix},\quad \psi_2{}^+=\begin{bmatrix}0\\\frac{1}{2}\sqrt{3}\sin\theta\\\frac{1}{2}\sin\theta\, e^{-2i\phi}\\-\cos\theta\, e^{-i\phi}\end{bmatrix};$$

$$E^-(\mathbf{k})=(A-B)k^2: \tag{2.8}$$

$$\psi_1{}^-=\begin{bmatrix}\cos\theta\, e^{-i\phi}\\-\frac{1}{2}\sin\theta\, e^{2i\phi}\\\frac{1}{2}\sqrt{3}\sin\theta\\0\end{bmatrix},\quad \psi_2{}^-=\begin{bmatrix}\frac{1}{2}\sin\theta\, e^{-2i\phi}\\\cos\theta\, e^{i\phi}\\0\\\frac{1}{2}\sqrt{3}\sin\theta\end{bmatrix}.$$

If the warping of the energy surfaces is neglected, the $E^+(\mathbf{k})$ and $E^-(\mathbf{k})$ in Eq. (2.8), with $B>A>0$, represent the energy spectrum for the conduction and valence bands, respectively, near the degenerate edge of α-Sn. The spinor functions in (2.8) then describe the spatially periodic part of the Bloch function for those states in terms of the four basis functions of the matrix H in (2.2).[9] Therefore from (2.8) we can obtain the overlap integral between the spatially periodic part of two Bloch functions belonging to the valence band with wave vector $\mathbf{k}$ and the conduction band with wave vector $\mathbf{k}+\mathbf{q}$ as follows:

$$\langle\mathbf{k},v|e^{-i\mathbf{q}\cdot\mathbf{r}}|\mathbf{k}+\mathbf{q},c\rangle=\tfrac{1}{2}\sqrt{3}\frac{q\sin\theta\, e^{i\phi}}{[k^2+q^2+2kq\cos\theta]^{1/2}}. \tag{2.9}$$

Here θ and ϕ specify the polar and azimuthal angles, respectively, of $\mathbf{k}$ with respect to $\mathbf{q}$; $\mathbf{q}$ has been taken as parallel to the (001) direction for simplicity.

III. CALCULATION OF DIELECTRIC CONSTANT

We can now evaluate $\epsilon(\mathbf{q})$ based on (2.1), using the matrix element in (2.9) and the energy spectrum for the two relevant bands given in (2.8). However, since the matrix element is evaluated by the $\mathbf{k}\cdot\mathbf{p}$ perturbation method and is only valid for states in the immediate vicinity of the band edge, we only calculate $\epsilon(\mathbf{q})$ in the limit of $\mathbf{q}\rightarrow 0$. If we change the summation over $\mathbf{k}$ in (2.1) into an integration over $\mathbf{k}$, with $\mathbf{q}$ in the (001) direction, and use the integration variables $\mu=\cos\theta$ and $x=k/q$, we have

$$\epsilon(q)=1+\frac{3e^2}{\pi(A+B)q}\int_0^{x_m}\int_{-1}^{1}dxd\mu \times\frac{x^2(1-\mu^2)}{(1+2x\mu+x^2)(1+2x\mu+\eta x^2)}, \tag{3.1}$$

where

$$\eta=2B/(A+B),$$

and the upper limit $x_m=k_m/q$, k_m being the radius of a sphere in k space which is equal to the Brillouin zone in volume. The double integral in (3.1) is evaluated as a power series in $1/x_m$ like

$$C_0+C_1(1/x_m)+\cdots,$$

with

$$C_0=[1/(\eta-1)] \times[\tfrac{1}{4}\pi^2-(1-\tfrac{1}{2}\eta)\pi\sin^{-1}(1/\eta^{1/2})-\tfrac{1}{2}\pi(\eta-1)^{1/2}]$$

and

$$C_1=-4/3\eta$$

for $\eta>1$. Hence we have

$$\epsilon(q)=\epsilon_0(1+\lambda/q),\quad q\rightarrow 0 \tag{3.2}$$

with

$$\epsilon_0=1-\frac{8e^2}{\pi\hbar^2k_m}\frac{m_e{}^*m_h{}^*}{m_e{}^*+m_h{}^*} \tag{3.3}$$

and

$$\lambda=\frac{3e^2m_h{}^*}{\hbar^2\epsilon_0}\left[\tfrac{1}{2}\pi-\left(\frac{m_h{}^*-m_e{}^*}{m_h{}^*}\right)\times\sin^{-1}\left(\frac{m_h{}^*}{m_h{}^*+m_e{}^*}\right)^{1/2}-\left(\frac{m_e{}^*}{m_h{}^*}\right)^{1/2}\right], \tag{3.4}$$

where we have put $A+B=\hbar^2/2m_e{}^*$ and $B-A=\hbar^2/2m_h{}^*$, $m_e{}^*$ and $m_h{}^*$ being the electron and hole effective mass, respectively.

For α-Sn, taking the density-of-states effective masses

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[8] We take $N=3B$. For the case $N=-3B$, the eigenfunctions should have different phases from the ones in (2.8).

[9] The explicit form of the four basis functions can be found in Ref. 7.

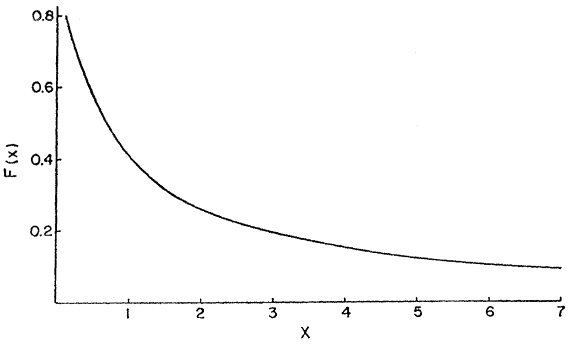

FIG. 1. The impurity potential is modified from the Coulomb form. The modulation function $F(x)$ is shown here.

$m_e^*=0.024m$,[10] $m_h^*=0.26m$,[11] and $k_m=0.85$ Å^{-1}, we get $\epsilon_0=0.88$ and $\lambda=0.18$ Å^{-1}. Since $\epsilon_0<1$, it looks as if the electrons would antishield any external charge. However, the value for ϵ_0 must be modified because of the contributions from other bands as well as from regions of **k** space not covered by the $\mathbf{k}\cdot\mathbf{p}$ expansion. This will be discussed in Sec. IV.

IV. SCREENING OF IMPURITY CHARGE

Now we discuss the screening of the impurity charge. If we assume a donor impurity with one excess charge, we can obtain the screened Coulomb potential by making the following Fourier transform:

$$V(\mathbf{r})=-\frac{e^2}{2\pi^2}\int d^3q\, e^{i\mathbf{q}\cdot\mathbf{r}}\frac{1}{\epsilon(\mathbf{q})q^2}. \tag{4.1}$$

Since we are interested in the tail of the screened potential, the dielectric function $\epsilon(\mathbf{q})$ in (4.1) can be taken as that given in (3.2). Then (4.1) leads to the following:

$$V(\mathbf{r})=-(e^2/\epsilon_0 r)F(\lambda r), \tag{4.2}$$

where the function F is given by

$$F(x)=\cos x[1-(2/\pi)\,\mathrm{Si}(x)]+(2/\pi)\sin x\,\mathrm{Ci}(x). \tag{4.3}$$

In (4.3), the functions $\mathrm{Si}(x)$ and $\mathrm{Ci}(x)$ are sine and cosine integrals defined by

$$\mathrm{Si}(x)=\int_0^x \frac{\sin t}{t}dt$$

and

$$\mathrm{Ci}(x)=-\int_x^\infty \frac{\cos t}{t}dt.$$

We plot in Fig. 1 the function $F(x)$. We can see that $F(x)$ is a slowly decreasing function of x. In other words, the screening is really not very effective.

In α-Sn, the contributions to the dielectric constant from other interband couplings remove the antishielding discussed in Sec. III and make ϵ_0 about 24.[12] Hence the actual value of the constant λ should be around 0.0066 Å^{-1}. By looking at Fig. 1, the value of $F(x)$ at $x=1$ is about 0.4. In other words, at a distance of ~150 Å away from the impurity site the strength of the Coulomb potential is only reduced by a factor of about 2. We have previously studied the problem of formation of impurity resonances in a zero-gap semiconductor with the impurity charge screened only by the dielectric constant ϵ_0 (plus a δ-function interaction representing the central-cell correction[13]). Owing to the ineffectiveness of the additional screening that we are discussing here, we do not anticipate any major modifications to the qualitative conclusions that we have reached there.

The $1/q$ singularity in the dielectric screening should also effect the transport properties in the low-temperature region when the ionized-impurity scattering dominates the phonon scattering. For example, we can expect the electron mobility to depend on the donor concentration. As the donor concentration decreases, the dielectric function (less the contribution from free carriers) approaches the form $\epsilon_0(1+\lambda/q)$ described in this paper. This means that the screening of bare impurity form factors is enhanced relative to what is expected from a free-carrier model as pertains in an ordinary semiconductor with sufficient doping to produce a degenerate carrier distribution. As a result, we expect a concomitant increase in the carrier mobility. An experimental study of the concentrational dependence of the carrier mobility in α-Sn has been made by Lavine and Ewald.[14] However, the data were analyzed phenomenologically on the assumption of a concentration-dependent dielectric constant. Nevertheless, their results strongly suggest that just such a sharp mobility enhancement was observed.

Part of this work has been reported elsewhere.[15]

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