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Effect of Nonparabolic Band Structure on Longitudinal Magnetoacoustic Phenomena

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The effect of nonparabolic band structure on the propagation of ultrasound in a semiconductor such as n -type InSb in the presence of longitudinal magnetic fields is discussed using a quantum treatment which is valid at high frequencies and in strong magnetic fields. The absorption coefficient and sound velocity for ultrasound propagating parallel to the magnetic field are found to change with magnetic field. This dependence on magnetic field arises solely from the nonparabolicity of the energy bands and would be in addition to any magnetic field dependence due to a field-dependent relaxation time. A numerical calculation is performed for the case of n -type InSb and a comparison is made with the experimental results of Nill and McWhorter.

I. INTRODUCTION

Recent experiments^{1, 2} in n -type InSb have found a magnetic field dependence of the absorption coefficient and the sound velocity for ultrasound propagating parallel to a magnetic field. Classically, the absorption of ultrasound propagating in a longitudinal magnetic field should be independent of magnetic field,^{3, 4} and this should be true even in the quantum regime for a model assuming parabolic energy bands and an energy-independent relaxation time.⁵ Jacoboni and Prohofska⁶ have shown that an energy- and magnetic-field-dependent relaxation time τ can give rise to a magnetic field dependence of the ultrasonic absorption in a longitudinal magnetic field and have tried to explain Nill and McWhorter's experimental results on this basis. In this paper, we show that the nonparabolicity of the band structure in a semiconductor⁷ like n -type InSb can lead to a change in the longitudinal magnetoacoustic absorption and the sound velocity in strong magnetic fields even when the magnetic field dependence of τ is neglected.

In our calculations we assume a nonparabolic model for the electronic energy bands and piezoelectric coupling between the acoustic wave and the conduction electrons. We also assume that the semiconductor is nondegenerate. The longitudinal ac conductivity is calculated using a quantum treatment which is valid for strong magnetic fields and high frequencies. Since we are interested in the high-frequency region $ql \gg 1$, the effect of collisions

is neglected. In Sec. II we present the calculation of the longitudinal ac conductivity for nonparabolic bands, and in Sec. III we present the numerical results for the absorption coefficient and sound velocity in n -type InSb. The discussion of the results using the nonparabolic model is given in Sec. IV, and comparison is made both with the results of the parabolic model and the experiments.

II. LONGITUDINAL CONDUCTIVITY FOR NONPARABOLIC BAND STRUCTURE

In the nonparabolic model, the relation between the energy and wave vector of an electron is⁸

$$E \left(1 + \frac{E}{E_g} \right) = \frac{p^2}{2m^*}, \quad (1)$$

where E_g is the energy gap between the conduction and valence bands and m^* is the effective mass of the electrons, which for our purpose we will take to be isotropic. The effective Hamiltonian for our system can be obtained by replacing \vec{p} by $\vec{p} - (e/c)\vec{A}$ in Eq. (1), where \vec{A} is the vector potential. For electrons in a uniform magnetic field directed along the z direction, the energy eigenvalue equation takes the form

$$E \left(1 + \frac{E}{E_g} \right) \psi = \frac{1}{2m^*} \left[P_x^2 + \left(P_y - \frac{eB}{c}x \right)^2 + P_z^2 \right] \psi, \quad (2)$$

where we have used the Landau gauge for the vector potential $\vec{A}_0 = (0, Bx, 0)$. This equation is identical to that for free electrons in a magnetic field and

yields the results

$$\psi_{kn} = e^{i(k_y y + \frac{1}{2} k_x^2 x)} \phi_n [x - (\hbar c / eB) k_y] \quad (3)$$

for the eigenfunctions and

$$E_{kn} = -\frac{E_g}{2} \left\{ 1 - \left[1 + \frac{4}{E_g} \left((n + \frac{1}{2}) \hbar \omega_c + \frac{\hbar^2 k_x^2}{2m^*} \right) \right]^{1/2} \right\} \quad (4)$$

for the eigenvalues, where $\omega_c = eB/m^*c$ is the cyclotron frequency and $\phi_n(x)$ is the harmonic oscillator function. When $(n + \frac{1}{2}) \hbar \omega_c \hbar^2 k_x^2 / 2m^* \ll E_g$, the energy eigenvalues reduce to those obtained using the parabolic model for the band structure. On the other hand, in strong magnetic fields $\hbar \omega_c \simeq E_g$ and the energy levels of the electrons are quite different from those that would be predicted by using the parabolic model.

The interaction of the electrons with the acoustic wave can be taken into account via the vector potential $\vec{A}_1 = \vec{A}_{10} e^{i(\vec{q} \cdot \vec{r} - \omega t)}$ which arises from the self-consistent piezoelectric field accompanying the sound wave. To first order in \vec{A}_1 the Hamiltonian is

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1, \quad (5)$$

where

$$\mathcal{H}_0 \psi_{kn} = E_{kn} \psi_{kn}$$

and

$$\mathcal{H}_1 = (e/2c)(\vec{v} \cdot \vec{A}_1 + \vec{A}_1 \cdot \vec{v}). \quad (6)$$

Here \vec{v} is the velocity operator for the unperturbed Hamiltonian $\vec{v} = -(i/\hbar)[\vec{r}, H_0]$. Using the effective Hamiltonian for the nonparabolic model, we find that

$$v_x = (1 + 2\mathcal{H}_0/E_g)^{-1} P_x/m^*, \quad (7a)$$

$$v_y = (1 + 2\mathcal{H}_0/E_g)^{-1} (P_y - eBx/c)/m^*, \quad (7b)$$

$$v_z = (1 + 2\mathcal{H}_0/E_g)^{-1} P_z/m^*. \quad (7c)$$

To obtain the components of the conductivity tensor we must first calculate the electron current density induced by the piezoelectric field. Following the same procedure as described in an earlier paper,⁹

we solve the equation of motion for the density operator ρ ,

$$i\hbar \frac{\partial \rho}{\partial t} = [\mathcal{H}, \rho], \quad (8)$$

by expanding the operator $\rho = \rho_0 + \rho_1$, where ρ_0 is the unperturbed density operator and linearizing the equation of motion (8). Taking the matrix elements of the linearized equation of motion in the representation (3) and (4), we find that

$$\langle k'n' | \rho_1 | kn \rangle = \frac{(f_{k'n'} - f_{kn}) \langle k'n' | H_1 | kn \rangle}{E_{k'n'} - E_{kn} - \hbar\omega}, \quad (9)$$

where

$$f_{kn} = \langle kn | \rho_0 | kn \rangle = n_0 e^{-\theta E_{kn}} / \sum_{kn} e^{-\theta E_{kn}}$$

is the Boltzmann distribution since we have assumed a nondegenerate semiconductor, n_0 is the electron density, and $\theta = 1/k_B T$. The electron current density is

$$\vec{J} = \text{Tr}(\rho \vec{J}_{op}) = \sum_{k'n'n} \langle k'n' | \rho | kn \rangle \langle kn | \vec{J}_{op} | k'n' \rangle, \quad (10)$$

where the current-density operator to first order in \vec{A}_1 is

$$\vec{J}_{op} = -\frac{e}{2} \left[\vec{v} - \left(1 + \frac{2\mathcal{H}_0}{E_g} \right)^{-1} \frac{e\vec{A}_1}{m^*c}, \delta(\vec{r} - \vec{r}_0) \right]_+, \quad (11)$$

and $[\]_+$ denotes the anticommutator.

Using the gauge where the scalar potential is zero, we find the following relation between the piezoelectric field and the vector potential \vec{A}_1 :

$$\vec{E} = (i\omega/c) \vec{A}_1. \quad (12)$$

In piezoelectric semiconductors, the coupling between the electrons and the acoustic wave is only important if the piezoelectric field induced by the wave is longitudinal. In our present case we are interested in an acoustic wave propagating parallel to the dc magnetic field so that the only component of the conductivity tensor of interest is σ_{xx} . Using Eqs. (3)-(12), we find that

$$\sigma_{xx}(q, \omega) = \frac{\omega_p^2}{4q^3 \hbar} \left(\frac{m^* \omega}{2\pi} \right)^{1/2} \left(\omega \sum_{n=0}^{\infty} a_n^{1/2} e^{-\theta E_g a_n/2} \right) \sum_{n=0}^{\infty} a_n e^{-\theta/2 E_g a_n} \left\{ w \left[- \left(\frac{\hbar^2 \theta}{2m^* a_n} \right)^{1/2} \left(\frac{q}{2} - \frac{m^* a_n \omega}{\hbar q} \right) \right] \right. \\ \left. - w \left[+ \left(\frac{\hbar^2 \theta}{2m^* a_n} \right)^{1/2} \left(\frac{q}{2} + \frac{m^* a_n \omega}{\hbar q} \right) \right] \right\}, \quad (13)$$

where

$$\omega_p = (4\pi n_0 e^2/m^*)^{1/2}$$

is the plasma frequency,

$$a_n = [1 + (4\hbar\omega_c/E_g)(n + \frac{1}{2})]^{1/2},$$

and

$$w(z) = e^{-z^2} \operatorname{erfc}(-iz)$$

is a function related to the complementary error function.¹⁰ In obtaining the above result, we have used the exponential cutoff of k_z provided by the Boltzmann distribution to expand Eq. (4),

$$E_{kn} \simeq -\frac{1}{2}E_g + \frac{1}{2}E_g a_n + \hbar^2 k_z^2 / 2m^* a_n, \quad (14)$$

since

$$(\hbar k_{z\max})^2 / 2m^* \simeq k_B T \ll E_g$$

for InSb at the low temperatures in which we are interested ($T < 100^\circ\text{K}$).

The relation between the absorption coefficient $\alpha_{||}$ and the longitudinal conductivity is given by⁴

$$\alpha_{||} = -\frac{4\pi\beta^2 q}{\rho\epsilon v_s^2} \operatorname{Im} \left(\frac{1}{1 - 4\pi\sigma_{zz}/i\omega\epsilon} \right), \quad (15)$$

where ρ is the density of the material, ϵ is the static dielectric constant, v_s is the sound velocity, and β is an appropriate piezoelectric constant. In a cubic crystal like InSb, the only component of the piezoelectric tensor which is nonvanishing is β_{14} .³ For \vec{q} parallel to the (110) direction $\beta = \beta_{14}$, while for \vec{q} parallel to the (111) direction $\beta = (2/\sqrt{3})\beta_{14}$ for waves which induce longitudinal electric fields.

The change in the sound velocity due to the interaction between the ultrasound and the conduction electrons is also related to the longitudinal conductivity⁴

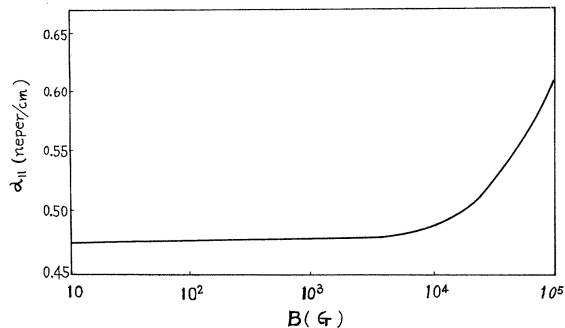


FIG. 1. Absorption coefficient $\alpha_{||}$ as a function of dc magnetic field B for nonparabolic band structure in n -InSb at $\omega = 10^{11}$ rad/sec, $T = 10^\circ\text{K}$, $q \parallel (111)$.

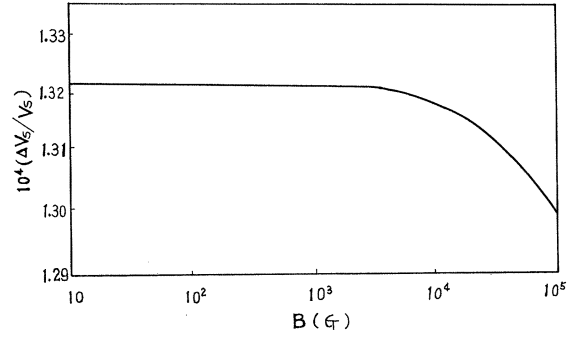


FIG. 2. Change in the sound velocity as a function of dc magnetic field B for nonparabolic band structure in n -InSb at $\omega = 10^{11}$ rad/sec, $T = 10^\circ\text{K}$, $q \parallel (111)$.

$$\frac{\Delta v_s}{v_s} = \frac{2\pi\beta^2}{\rho\epsilon v_s^2} \operatorname{Re} \left(\frac{1}{1 - 4\pi\sigma_{zz}/i\omega\epsilon} \right). \quad (16)$$

Therefore, if one knows the longitudinal conductivity σ_{zz} , one can obtain the absorption coefficient and the change in the sound velocity.

III. NUMERICAL RESULTS

From Eqs. (13), (15), and (16), it can be seen that $\alpha_{||}$ and $\Delta v_s/v_s$ will depend upon the magnetic field when we use the nonparabolic model for the energy bands of a semiconductor. For comparison, the result for the longitudinal conductivity using the parabolic model,^{1,5}

$$\sigma_{zz} = \frac{\omega_p^2 \omega}{4\hbar q^3} \left(\frac{m^* \theta}{2\pi} \right)^{1/2} \times \left\{ w \left[- \left(\frac{\hbar^2 \theta}{2m^*} \right)^{1/2} \left(\frac{q}{2} - \frac{m^* \omega}{\hbar q} \right) \right] - w \left[+ \left(\frac{\hbar^2 \theta}{2m^*} \right)^{1/2} \left(\frac{q}{2} + \frac{m^* \omega}{\hbar q} \right) \right] \right\}, \quad (17)$$

is independent of magnetic field. We can readily see that (13) will reduce to (17) if $\hbar\omega_c \ll E_g$, so that at low magnetic fields, the result using a parabolic model for the energy bands should be valid. On the other hand, in strong magnetic fields such that $\hbar\omega_c \simeq E_g$, the nonparabolicity of the energy bands leads to qualitatively different results.

As a numerical example, we shall consider the absorption of ultrasound and the change of sound velocity in n -type InSb at high frequencies and at low temperatures. The relevant values of the parameters for this material are $n_0 = 1.75 \times 10^{14} \text{ cm}^{-3}$, $m^* = 0.013m_0$, $\epsilon = 18$, $\beta_{14} = 1.8 \times 10^4 \text{ esu/cm}^2$, $E_g = 0.2 \text{ eV}$, $\rho = 5.8 \text{ g/cm}^3$, and $v_s = 4 \times 10^5 \text{ cm/sec}$. The results for $\alpha_{||}$ and the change in sound velocity as functions of magnetic field are shown in Figs.

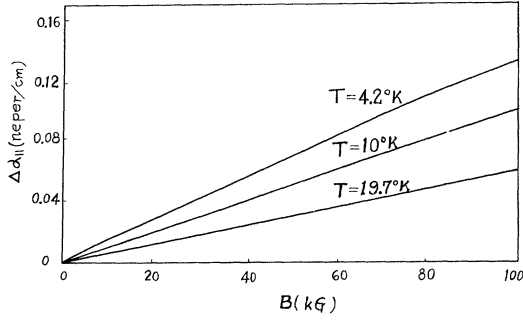


FIG. 3. Change in the attenuation $\Delta\alpha_{||}$ as a function of magnetic field in n -InSb at $\omega = 5.655 \times 10^{10}$ rad/sec and $q_{||}$ (111) for three different temperatures.

1 and 2, for $\omega = 10^{11}$ rad/sec, $T = 10^\circ\text{K}$, and propagation parallel to the (111) direction. It can be seen that at low magnetic field both $\alpha_{||}$ and $\Delta v_s/v_s$ are independent of the field, while at high fields, $\alpha_{||}$ increases and $\Delta v_s/v_s$ decreases with the field. In fact, the absorption coefficient is about 30% higher at a magnetic field of 100 kG than would be predicted using the parabolic model.

For comparison with the experiments of Nill and McWhorter, we have plotted $\Delta\alpha_{||} = \alpha_{||}(B) - \alpha_{||}(0)$ as a function of magnetic field for three different values of the temperature and at a frequency of 9 GHz in Fig. 3. As can be seen from Fig. 3, $\Delta\alpha_{||}$ increases more rapidly with magnetic field when the temperature is lowered. In Fig. 4, $\Delta\alpha_{||}$ is shown as a function of magnetic field for three different frequencies and at a temperature of 10°K . The reason that $\Delta\alpha_{||}$ has a maximum as a function of frequency is due to the breakdown of screening in a semiconductor of this carrier density in the microwave frequency region. In Figs. 5 and 6 $[\Delta v_s(B) - \Delta v_s(0)]/v_s$ is shown as a function of magnetic field for three different temperatures and frequencies. Again the change from the zero-field value becomes larger as the temperature decreases and has a maximum as a function of frequency in

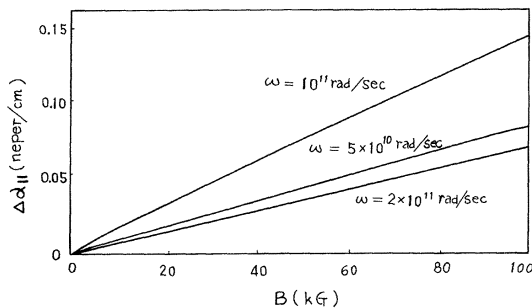


FIG. 4. Change in the attenuation $\Delta\alpha_{||}$ as a function of magnetic field in n -InSb at $T = 10^\circ\text{K}$ for three different frequencies.

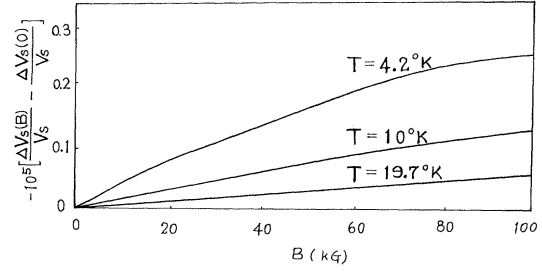


FIG. 5. Difference of the change in sound velocity as a function of magnetic field in n -InSb at $\omega = 5.655 \times 10^{10}$ rad/sec for three different temperatures.

the microwave ultrasonic region.

IV. DISCUSSION

The calculations presented here show that the nonparabolic band structure of a semiconductor such as n -type InSb can lead to a magnetic field dependence of the acoustic absorption and the sound velocity for waves propagating parallel to the magnetic field. This is in contrast to the results using a parabolic model for the band structure, which predict no magnetic field dependence of the acoustic absorption or the sound velocity in a longitudinal magnetic field. The deviations from the predictions of the parabolic model become important when the spacing between the Landau levels, $\hbar\omega_c$, becomes comparable to the energy gap E_g . The parameter $\hbar\omega_c/E_g$ becomes equal to unity at a magnetic field of about 200 kG. Under these conditions, the dependence of the energy of the conduction electron on magnetic field using the nonparabolic model differs from what it would be using the parabolic model. It is this dependence of electron energy on magnetic field which leads to the magnetic field dependence of $\alpha_{||}$ and v_s for the case of nonparabolic bands.

The use of the nonparabolic model predicts an in-

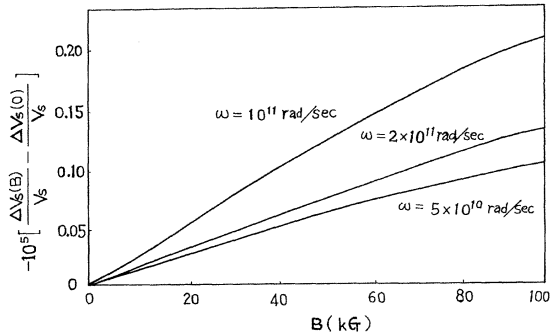


FIG. 6. Difference of the change in sound velocity as a function of magnetic field in n -InSb at $T = 10^\circ\text{K}$ for three different frequencies.

crease in the absorption of ultrasound with increasing magnetic field. This is in qualitative agreement with the experiments^{1, 2} although the theory does not agree with the present experiment in all the details. For instance, the increase in absorption predicted is only about 20% of what is experimentally observed. However, since Jacoboni and Prohofsky have predicted a similar effect because of a magnetic field dependent τ , the experiments may indicate that both effects play an important role. In addition, Nill and McWhorter estimated that in their experiments ql was about 5. Since the effect of the magnetic field on the relaxation time would be to reduce its value below that at zero field,⁶ the theory presented here, which neglects the effect of collisions, would cease to be valid as one went to higher fields. On the other hand, as we went to higher frequencies, we would expect the theory to be valid at higher magnetic fields, as the parameter ql scales both with frequency and relaxation time.

The change of the sound velocity with magnetic field using the nonparabolic model is of the same magnitude as that observed experimentally. The sound velocity decreases because of an increase in the screening of the piezoelectric field due to the increase in σ_{xx} with magnetic field. This increased screening does not reduce the absorption because of a greater increase in the number of carriers

which interact resonantly with the ultrasound. The effect of the nonparabolicity in the band structure is to introduce an energy, and therefore, a magnetic-field-dependent effective mass for the electrons. This effective mass for electrons in a Landau level of quantum number n is m^*a_n . The effective mass introduced in this manner increases with magnetic field and leads to an increase in the density of states for those electrons which are in resonance with the sound wave. Since the ac conductivity for the electron increases with decreasing temperature, the changes in $\alpha_{||}$ and the sound velocity will become larger as the temperature is lowered.

In conclusion, our calculations show that the effect of nonparabolicity on the longitudinal magneto-absorption of ultrasound is important and must be taken into account in any theory of ultrasonic effects in n -type InSb. The change in the absorption with magnetic field due to the nonparabolicity is smaller than what is observed experimentally at 9 GHz, but the effects of nonparabolicity should become more important at higher frequencies where the field-dependent relaxation time can be neglected. The effect of the nonparabolicity may explain the increase in absorption with field observed experimentally at the higher temperatures where the field dependence of the relaxation time would be expected to be less important.

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