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Coupling mechanisms of acoustic second-harmonic generation in piezoelectric semiconductors

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Abstract. Acoustic second-harmonic generation is studied in non-degenerate piezoelectric semiconductors, such as n-type InSb, with a uniform DC magnetic field $\boldsymbol{B}$ directed along the acoustic wave. The effect of electron scattering in solids has been taken into consideration, so the electron relaxation time cannot be neglected. Coupling mechanisms for the electron–phonon interaction are taken into account in this investigation through both deformation potential and piezoelectric couplings. It is found that the second-harmonic generation due to the piezoelectric coupling appears to be comparable with that due to the deformation potential coupling only in the approximate range of frequencies $\omega = 6 \times 10^{10}$–$4 \times 10^{11}$ rad s^{-1}. Outside this range of frequencies, the deformation potential coupling becomes more significant than the piezoelectric coupling for the second-harmonic generation in semiconductors.

1. Introduction

The non-linear properties of semiconductors can be used to generate second harmonics in the microwave region. These non-linear properties are of interest in the sense of using them to generate higher harmonics of high-frequency signals (Chatterjee and Das 1983). In high-mobility semiconductors such as n-type InSb, the application of a strong magnetic field can crucially alter the behaviour of the electron–phonon interaction due to the non-parabolicity of the energy bands. Experimental results have indicated that the piezoelectric scattering is predominantly responsible for the electron energy relaxation and that the deformation potential scattering appears to play no significant role in the electron energy relaxation (Lifshitz *et al* 1966, Whalen and Westgate 1972). From the phenomenological theory, Spector (1974) showed that in intrinsic semiconductors and semimetals the harmonic generation due to the deformation potential coupling can become comparable with that arising from the piezoelectric coupling in a typical piezoelectric semiconductor. Hansen (1981) proposed a correct form of the velocity operator from the Hamiltonian operator to show that the Hall effect cannot be influenced by non-parabolicity in the limit of vanishing scattering. However, when the acoustic wave is propagating parallel to a DC magnetic field and when the electron scattering in solids is not neglected, the non-parabolicity of the energy bands leads of an enhancement of the

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magneto-acoustic absorption (Sutherland and Spector 1978). In this paper we investigate the acoustic second-harmonic generation in non-degenerate piezoelectric semiconductors such as n-type InSb by taking into account the effect of an electron relaxation time due to the scattering in semiconductors at low temperatures when the acoustic wave propagates longitudinally. The energy band structure of electrons is assumed to be non-parabolic. The effect of scattering cannot be neglected in real crystals, since there are sufficient imperfections to provide plenty of scattering even at low temperatures. The electron–phonon interaction in semiconductors is assumed to arise from both deformation potential and piezoelectric couplings in which self-consistent fields are produced accompanying acoustic waves. We use the Heisenberg equation of motion to correct the effect of the non-parabolic band structure of semiconductors.

In § 2 we present the theoretical development of our problem for a non-parabolic band structure in the presence of a DC magnetic field $\boldsymbol{B}$ by introducing an electron relaxation time. In § 3 the numerical analysis for n-type InSb is given together with a brief discussion.

2. Theoretical development

The Hamiltonian H_0 for an electron of the non-parabolic-band model in a uniform DC magnetic field $\boldsymbol{B}$ directed along the z axis can be written in the form (Wu and Spector 1972)

$$H_0(1 + H_0/E_g) = (1/2m^*)[p_x^2 + (p_y - eBx/c)^2 + p_z^2] \equiv F(p_x, p_y, p_z) \tag{1}$$

where m^* is the effective mass of electrons at the minimum of the conduction band and E_g is the energy gap between the conduction and valence bands. In equation (1) we have used the Landau gauge for the vector potential $\boldsymbol{A}_0 = (0, Bx, 0)$. The eigen-functions and eigenvalues for equation (1) can be expressed as (Wu and Spector 1972)

$$\Psi_{kn} = \exp(\mathrm{i}k_y y + \mathrm{i}k_z z)\Phi_n[x - (\hbar c/eB)k_y] \tag{2}$$

and

$$E_{kn} = -\tfrac{1}{2}E_g[\![1 - \{1 + (4/E_g)[(n + \tfrac{1}{2})\hbar\omega_c + \hbar^2 k_z^2/2m^*]\}^{1/2}]\!] \tag{3}$$

respectively, where k_y and k_z are the y and z components of the electron wave-vector $\boldsymbol{k}$, $\Phi_n(x)$ is the harmonic oscillator wavefunction and $\omega_c = |e|B/m^*c$ is the cyclotron frequency of electrons. E_{kn} is the energy of the system defined by $H_0\Psi_{kn} = E_{kn}\Psi_{kn}$.

The interaction of electrons with acoustic waves can be taken into account via the vector potential $\boldsymbol{A}_1 = \boldsymbol{A}_{10}\exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r} - \mathrm{i}\omega t)$, which arises from the self-consistent fields accompanying acoustic waves. Up to second order in $\boldsymbol{A}_1$ the Hamiltonian for an electron in the presence of the DC magnetic field and self-consistent fields can be written as

$$H = H_0 + H_1 + H_2 \tag{4}$$

where H_0 is the unperturbed Hamiltonian of electrons, and H_1 and H_2 are perturbed Hamiltonians of the first and second orders, respectively. Using the Heisenberg equation of motion, these perturbed Hamiltonians can be expressed as

$$H_1 = -(e/2c)(\boldsymbol{v}\cdot\boldsymbol{A}_1 + \boldsymbol{A}_1\cdot\boldsymbol{v}) \tag{5}$$

and

$$H_2 = \frac{e^2}{2c^2}\left(1 + \frac{H_0^{(r)} + H_0^{(l)}}{E_g}\right)^{-1}\left[\frac{\partial^2 F}{\partial p_i \partial p_j} A_{1i} A_{1j} - \frac{1}{2E_g}\left(1 + \frac{H_0^{(r)} + H_0^{(l)}}{E_g}\right)^{-2} \times \left(A_{1i}\frac{\partial F}{\partial p_i} + \frac{\partial F}{\partial p_i} A_{1i}\right)\left(A_{1j}\frac{\partial F}{\partial p_j} + \frac{\partial F}{\partial p_j} A_{1j}\right)\right] \tag{6}$$

respectively, where

$$\boldsymbol{v} = (1/\mathrm{i}\hbar)[\boldsymbol{r}, H_0] = (\partial F/\partial \boldsymbol{p})/[1 + (H_0^{(r)} + H_0^{(l)})/E_g]. \tag{7}$$

$H_0^{(r)}$ and $H_0^{(l)}$ are the right and left Hamiltonian operators such that $H_0^{(r)}\Psi_{kn} = E_{kn}\Psi_{kn}$ and $\Psi_{k'n'}^* H_0^{(l)} = E_{k'n'}\Psi_{k'n'}^*$, respectively. Since the different quantum states can produce different eigenvalues, the right and left Hamiltonian operators cause an important non-linear effect to occur in the electron–phonon interaction, due to the non-parabolicity of energy bands in semiconductors.

The density matrix $\boldsymbol{\rho}$ can be expressed up to second order in the amplitude of acoustic waves:

$$\boldsymbol{\rho} = \boldsymbol{\rho}_0 + \boldsymbol{\rho}_1 + \boldsymbol{\rho}_2 \tag{8}$$

where $\boldsymbol{\rho}_0$ is independent of time, $\boldsymbol{\rho}_1$ varies as $\exp(-\mathrm{i}\omega t)$ and $\boldsymbol{\rho}_2$ varies as $\exp(-2\mathrm{i}\omega t)$. The quantum Liouville equation including the effect of scattering in solids can be expressed as (Sutherland and Spector 1978)

$$\partial\boldsymbol{\rho}/\partial t + (\mathrm{i}\hbar)[H, \boldsymbol{\rho}] = -(\boldsymbol{\rho} - \boldsymbol{\rho}_0)/\tau \tag{9}$$

where τ is the electron relaxation time due to the scattering in solids. The current density $\boldsymbol{J}$ can be obtained from (Spector 1966)

$$\boldsymbol{J} = \mathrm{Tr}(\boldsymbol{\rho}\cdot\boldsymbol{J}_{\mathrm{op}}) = \sum_{kk',nn'} \langle \boldsymbol{k}'n'|\boldsymbol{\rho}|\boldsymbol{k}n\rangle\langle \boldsymbol{k}n|\boldsymbol{J}_{\mathrm{op}}|\boldsymbol{k}'n'\rangle \tag{10}$$

where

$$\boldsymbol{J}_{\mathrm{op}} = -(e/2)[(\boldsymbol{v} + \boldsymbol{v}'), \delta(\boldsymbol{r} - \boldsymbol{r}_0)]_+ \tag{11}$$

with the velocity operator $\boldsymbol{v}' = (1/\mathrm{i}\hbar)[\boldsymbol{r}, (H_1 + H_2)]$ due to the electron–phonon interaction. The explicit expression for this velocity operator $\boldsymbol{v}'$ can be obtained from equations (5) and (6) as in the method we used in our previous work (Wu and Spector 1972). Using the gauge where the scalar potential is zero, the relation between the electric field and the vector potential is given by

$$\boldsymbol{E} = (\mathrm{i}\omega/c)\boldsymbol{A}_1. \tag{12}$$

From equations (2)–(12), one may obtain the current density in the form

$$J_i = \sigma_{ij}E_j + \tau_{ijk}E_jE_k \tag{13a}$$

for the piezoelectric coupling, and

$$J_i = \sigma_{ij}\left[E_j - \frac{\partial}{\partial x_j}\left(\frac{V_{lm}}{e}S_{lm}\right)\right] + \tau_{ijk}\left[E_j - \frac{\partial}{\partial x_j}\left(\frac{V_{lm}}{e}S_{lm}\right)\right]\left[E_k - \frac{\partial}{\partial x_k}\left(\frac{V_{np}}{e}S_{np}\right)\right] \tag{13b}$$

for the deformation potential coupling (Spector 1974), where σ_{ij} is the linear conductivity tensor, τ_{ijk} is the non-linear conductivity tensor, E_i is the induced self-consistent field,

S_{ij} is the strain tensor and V_{ij} is the deformation potential tensor of the electrons. In the present case we are interested in the acoustic wave propagating parallel to the DC magnetic field $\boldsymbol{B}$, so the only components of conductivity tensors that play an important role in second-harmonic generation will be those of σ_{zz} and τ_{zzz} (Wu and Spector 1972). These tensors can be expressed as

$$\sigma_{zz}(\boldsymbol{q}, \omega) = \frac{(\omega_p^*)^2}{4\pi i\omega n_0}\bigg(\sum_{k,n} f_{kn}\theta_{kn} - \frac{\hbar^2}{4m^*}\sum_{k,n}(\theta^{kn}_{k+q,n})^2(2k_z + q_z)^2 \times \frac{f_{kn} - f_{k+q,n}}{E_{k+q,n} - E_{kn} - \hbar(\omega + i\tau^{-1})}\bigg) \tag{14}$$

and

$$\tau_{zzz}(\boldsymbol{q}, \omega) = -\frac{3(\omega_p^*)^2 e q_z \hbar}{4\pi m^* \omega^2 n_0 E_g}\sum_{k,n} f_{kn}\theta^3_{kn} - \frac{(\omega_p^*)^2 e\hbar}{8\pi m^*\omega^2 n_0}\bigg(\sum_{k,n}\frac{(f_{kn} - f_{k+q,n})}{E_{k+q,n} - E_{kn} - \hbar(\omega + i\tau^{-1})} \times (\theta^{kn}_{k+q,n})^2(2k_z + q_z) + \tfrac{1}{2}\sum_{k,n}\frac{(f_{kn} - f_{k+2q,n})}{E_{k+2q,n} - E_{kn} - \hbar(2\omega + i\tau^{-1})} \times (\theta^{kn}_{k+2q,n})^2(2k_z + 2q_z) - \frac{\hbar^2}{4m^*}\sum_{k,n} G(\boldsymbol{k}, \boldsymbol{k} + 2\boldsymbol{q}, \boldsymbol{k} + \boldsymbol{q}; n) \times \theta^{kn}_{k+2q,n}\theta^{k+2q,n}_{k+q,n}\theta^{k+q,n}_{kn}(2k_z + q_z)(2k_z + 2q_z)(2k_z + 3q_z)\bigg) \tag{15}$$

where

$$G(\boldsymbol{k}, \boldsymbol{k} + 2\boldsymbol{q}, \boldsymbol{k} + \boldsymbol{q}; n) = \{f_{k+2q,n}[E_{k+q,n} - E_{kn} - \hbar(\omega + i\tau^{-1})] - f_{k+q,n}[E_{k+2q,n} - E_{kn} - \hbar(2\omega + i\tau^{-1})] + f_{kn}[E_{k+2q,n} - E_{k+q,n} - \hbar(\omega + i\tau^{-1})]\}[E_{k+2q,n} - E_{kn} - \hbar(2\omega + i\tau^{-1})]^{-1} \times [E_{k+2q,n} - E_{k+q,n} - \hbar(\omega + i\tau^{-1})]^{-1} \times [E_{k+q,n} - E_{kn} - \hbar(\omega + i\tau^{-1})]^{-1} \tag{16}$$

$$\theta_{kn} = (1 + 2E_{kn}/E_g)^{-1} \tag{17}$$

and

$$\theta^{kn}_{k'n'} = (1 + E_{kn}/E_g + E_{k'n'}/E_g)^{-1}. \tag{18}$$

The basic equation of motion for an elastic continuum is (Wu and Spector 1972)

$$d\partial^2\xi_i/\partial t^2 = \partial T_{ij}/\partial x_j \tag{19}$$

where

$$\boldsymbol{\xi} = \sum_n \boldsymbol{\xi}_{n0}\exp[in(\boldsymbol{q}\cdot\boldsymbol{r} - \omega t)]$$

is the displacement of acoustic waves, d is the density of material and T_{ij} is the stress tensor. When acoustic waves interact with electrons via the deformation potential and piezoelectric couplings, the stress–strain relation is given by (Johri and Spector 1977)

$$T_{ij} = C_{ijkl}S_{kl} - nV_{ij} - \beta_{ijk}E_k \tag{20}$$

where C_{ijkl} is the elastic tensor, β_{ijk} is the piezoelectric tensor and n is the electron charge density. From the equation of continuity, the charge density n and the electric current density $\boldsymbol{J}$ should satisfy

$$\nabla \cdot \boldsymbol{J} + \partial n/\partial t = 0. \tag{21}$$

In a piezoelectric material, the electric displacement induced by applying a strain can be expressed by (Spector 1966)

$$D_i = \varepsilon_{ij} E_j + 4\pi \beta_{ijk} S_{jk} \tag{22}$$

where ε_{ij} is the dielectric tensor. Since the off-diagonal components of ε_{ij} are zero except for in triclinic and monoclinic crystal structures (Cady 1964), we take ε_{ij} to have only diagonal components in the present case. The dielectric tensor ε_{ij} in this expression arises solely from the lattice contribution to the dielectric tensor, and therefore it is a scalar quantity ε.

Let the plane-wave solutions for the electromagnetic field and displacement up to second-harmonic generation be of the following forms:

$$\boldsymbol{E} = \boldsymbol{E}_{10} \exp[\mathrm{i}(\boldsymbol{q} \cdot \boldsymbol{r} - \omega t)] + \boldsymbol{E}_{20} \exp[2\mathrm{i}(\boldsymbol{q} \cdot \boldsymbol{r} - \omega t)] \tag{23}$$

$$\boldsymbol{\xi} = \boldsymbol{\xi}_{10} \exp[\mathrm{i}(\boldsymbol{q} \cdot \boldsymbol{r} - \omega t)] + \boldsymbol{\xi}_{20} \exp[2\mathrm{i}(\boldsymbol{q} \cdot \boldsymbol{r} - \omega t)]. \tag{24}$$

Then, from equations (13*a*), (13*b*), (19)–(24), and Maxwell's equations for a non-magnetic medium,

$$\nabla \times \boldsymbol{E} = -(1/c)\partial \boldsymbol{H}/\partial t \tag{25}$$

and

$$\nabla \times \boldsymbol{H} = (4\pi/c)\boldsymbol{J} + (1/c)\partial \boldsymbol{D}/\partial t \tag{26}$$

one can obtain the longitudinal amplitude of displacement in a longitudinal magnetic field for $\boldsymbol{q} \parallel [111]$ as

$$\xi_{2z0}^{(\mathrm{d})} \simeq \frac{q^2 V_{zz} \tau_{zzz}(\boldsymbol{q}, \omega) \xi_{1z0}^2}{4|e|(2\sigma_{zz}(2\boldsymbol{q}, 2\omega) - \sigma_{zz}(\boldsymbol{q}, \omega))} \tag{27}$$

due to the deformation potential coupling, and

$$\xi_{2z0}^{(\mathrm{p})} \simeq \frac{-4\pi \mathrm{i} q \omega \beta_{14} \tau_{zzz}(\boldsymbol{q}, \omega) \xi_{1z0}^2}{3^{1/2}(2\sigma_{zz}(\boldsymbol{q}, \omega) - \sigma_{zz}(2\boldsymbol{q}, 2\omega))(4\pi \mathrm{i} \sigma_{zz}(\boldsymbol{q}, \omega) + \omega\varepsilon)} \tag{28}$$

due to the piezoelectric coupling. The simple expressions obtained in equations (27) and (28) are approximated by using the fact that the sound velocity v_s is quite small compared with the velocity of light c. That is, some terms containing a factor of $(v_s/c)^2 \simeq 1.7 \times 10^{-10}$ or higher order can be neglected in our calculations. In here, V_{zz} is the deformation potential and β_{14} is the piezoelectric constant.

The acoustic intensity P_n is defined by (Tell 1964)

$$P_n = \tfrac{1}{2} d |\partial \boldsymbol{\xi}_{n0}/\partial t|^2 v_s = \tfrac{1}{2} d n^2 \omega^2 |\boldsymbol{\xi}_{n0}|^2 v_s \tag{29}$$

with

$$|\boldsymbol{\xi}_{20}|^2 = |\xi_{2z0}^{(\mathrm{d})}|^2 + |\xi_{2z0}^{(\mathrm{p})}|^2. \tag{30}$$

Therefore, the acoustic intensity in the second-harmonic generation due to the longitudinal polaristion for $\boldsymbol{q} \parallel [111]$ is given by

$$P_2/P_1^2 = (q^4 V_{zz}^2/2dv_s\omega^2 e^2)|\tau_{zzz}(\boldsymbol{q},\omega)/(2\sigma_{zz}(2\boldsymbol{q},2\omega) - \sigma_{zz}(\boldsymbol{q},\omega))|^2 + (2/3dv_s^3)|^2$$
$$\times (8\pi\beta_{14}/\varepsilon)^2|\tau_{zzz}(\boldsymbol{q},\omega)/(2\sigma_{zz}(\boldsymbol{q},\omega) - \sigma_{zz}(2\boldsymbol{q},2\omega))$$
$$\times (1 - 4\pi\sigma_{zz}(\boldsymbol{q},\omega)/\mathrm{i}\omega\varepsilon)|^2. \tag{31}$$

3. Numerical analysis and discussion

As a numerical example we consider the propagation of acoustic waves travelling to a DC magnetic field $\boldsymbol{B}$ in n-type InSb for a simple case with a constant relaxation time due to the scattering in semiconductors. The relevant values of physical parameters for this material are (Nill and McWhorter 1966, Wu and Spector 1972, Sutherland and Spector 1978) $n_0 = 1.75 \times 10^{14}\,\mathrm{cm^{-3}}$, $m^* = 0.013m_0$ (m_0 is the mass of free electron), $\varepsilon = 18$, $\beta_{14} = 1.8 \times 10^4\,\mathrm{esu\,cm^{-2}}$, $E_g = 0.2\,\mathrm{eV}$, $V_{zz} = 4.5\,\mathrm{eV}$, $d = 5.8\,\mathrm{g\,cm^{-3}}$, $\tau = 10^{-12}\,\mathrm{s}$ and $v_s = 4 \times 10^5\,\mathrm{cm\,s^{-1}}$. The ratio of the acoustic intensity in the second harmonic to the square of the intensity in the fundamental as a function of frequency at $T = 4.2\,\mathrm{K}$ and $B = 50\,\mathrm{kG}$ for combining both deformation potential and piezoelectric couplings is shown in figure 1. It is found that the acoustic intensity of the second harmonic decreases

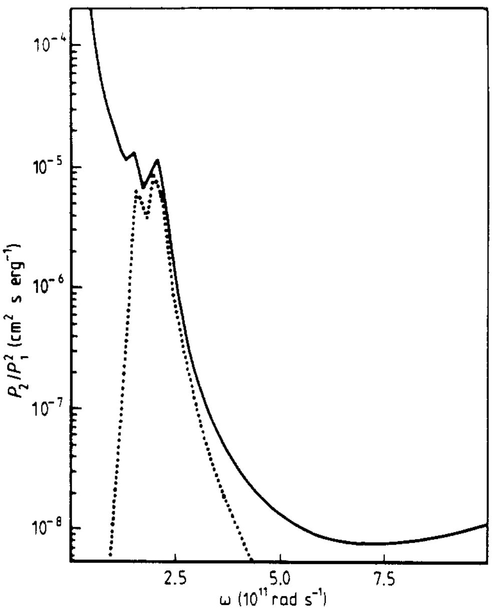

Figure 1. The ratio of the acoustic intensity in the second harmonic to the square of the acoustic intensity in the fundamental as a function of frequency in n-type InSb at $T = 4.2\,\mathrm{K}$ and $B = 50\,\mathrm{kG}$ for combining both deformation potential and piezoelectric couplings. The dotted curve indicates numerical results for piezoelectric coupling alone.

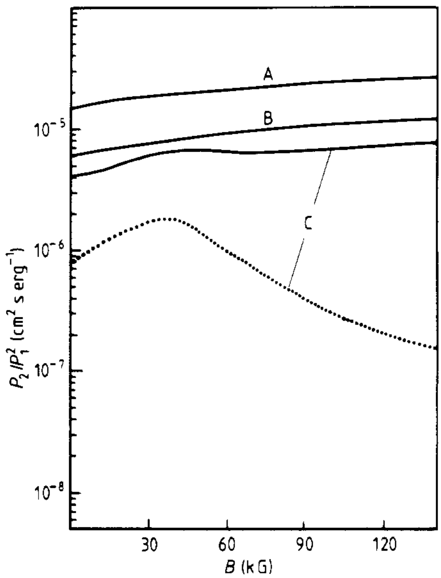

Figure 2. The ratio of the acoustic intensity in the second harmonic to the square of the acoustic intensity in the fundamental as a function of DC magnetic field in n-type InSb at $\omega = 10^{11}\,\mathrm{rad\,s^{-1}}$ for combining both deformation potential and piezoelectric couplings. $T =$ (A) 4.2, (B) 10 and (C) $T = 19.7\,\mathrm{K}$. The dotted curve indicates numerical results for piezoeletric coupling alone at $T = 19.7\,\mathrm{K}$.

rapidly with frequency when frequencies are below 5×10^{11} rad s^{-1}. After passing the minimum point around $\omega = 6 \times 10^{11}$ rad s^{-1}, the acoustic intensity of the second harmonic increases slowly with frequency. It can be seen that there are some local maximum points in the neighbourhood of frequencies $\omega = 10^{11}$–2×10^{11} rad s^{-1}. When the frequency is in the range $\omega = 6 \times 10^{10}$–$4 \times 10^{11}$ rad s^{-1}, the electron–phonon interaction of the piezoelectric coupling becomes comparable with that of the deformation potential coupling as shown by the dotted curve. Thus these peaks arise from the self-consistent field induced by the piezoelectric coupling. We plot the ratio of the acoustic intensity in the second harmonic to the square of the intensity in the fundamental as a function of the magnetic field at $\omega = 10^{11}$ rad s^{-1} for combining both deformation potential and piezoelectric couplings in figure 2. We can see that at very low temperatures the acoustic intensity of the second harmonic changes monotonically with the magnetic field. However, when the temperature increases, there is a maximum due to the piezoelectric coupling. From our numerical results presented here, we predict that the deformation potential coupling will become more significant than the piezoelectric coupling when we take into account the relaxation time of scattering in solids for the quantum mechanical treatment. However, the electron–phonon interaction of piezoelectric coupling becomes significant when the frequency lies in the microwave region.

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