



Terahertz absorption by electrons and confined acoustic phonons in free-standing quantum wells

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The acoustic phonon confinement in a free-standing quantum well (FSQW) results in an acoustic phonon energy quantization. Typical quantization energies are in the terahertz frequency range. Free electrons may absorb electromagnetic waves in this frequency range if they emit or absorb acoustic phonons. Therefore, the terahertz absorption reveals the characteristic features of the acoustic phonon spectrum in free-standing structures. We have calculated the absorption coefficient of an electromagnetic wave by free electrons in a FSQW in the terahertz frequency range. We took into account a time dependent electric field, an exact form of the acoustic phonon spectrum and eigenmodes, and electron interactions with confined acoustic phonons through the deformation potential. We demonstrate numerical results for GaAs FSQW of width 100 Å at low lattice temperatures in the frequency range 0.1–1 THz. The absorption coefficient exhibits several structures at frequencies corresponding to the lowest acoustic phonon modes. These features occur due to absorption of photons by electrons, which is accompanied by the emission of corresponding acoustic phonons.

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1. Introduction

Electromagnetic wave absorption under conditions when the photon energy, $\hbar\Omega$, is comparable with the average kinetic energy of electrons, $\bar{\epsilon}$, is a useful tool for investigating various types of interactions in solids. In this case, the spectral dependence of the absorption coefficient depends on the details of the scattering processes and it carries information about such processes, as opposite to the quasiclassical case $\hbar\Omega \ll \bar{\epsilon}$, where the Drude formula is valid. Measurements of the absorption coefficient in the far-infrared region have been used to investigate electron scattering in bulk semiconductors [1]. The light absorption by free carriers with the participation of optical phonons in quasi-two-dimensional systems have been studied in Ref. [2]. To the best of our knowledge, so far there has been no work devoted to light absorption by two-dimensional (2D) electrons with participation of acoustic phonons.

It is well known that acoustic phonons in heterostructures have confined modes which interact with photons in a specific way. This phenomenon is much stronger in the case of free-standing quantum wells (FSQWs) [3,4] or unsupported thin metallic films [5]. A typical energy of acoustic phonons in such structures is about $\hbar s/a$, where a is the width of the quantum well and s is the acoustic phonon velocity. For typical values $a = 100$ Å, $s = 5 \times 10^5$ cm s⁻¹, the phonon energy is equal to 1 meV (or about 0.25 THz). It is a small energy in the case of high lattice temperatures; however,

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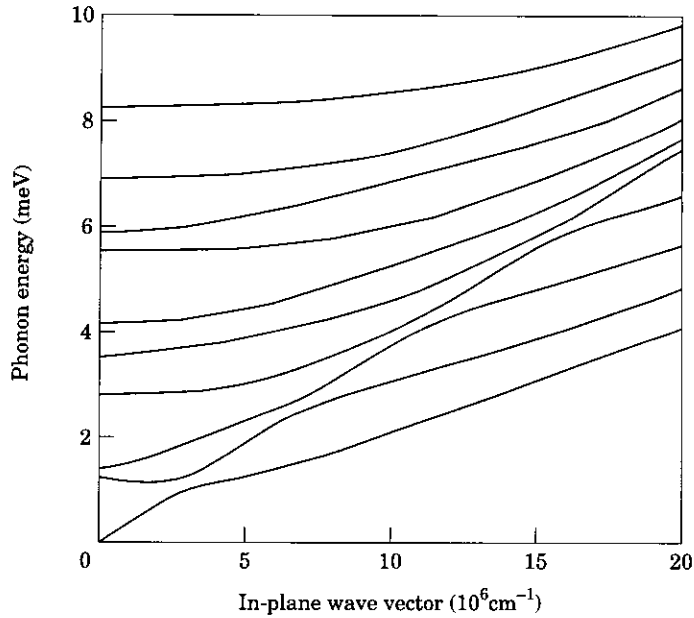


Fig. 1. The dispersion relation for dilatational modes in a GaAs FSQW of width 100 Å. Ten branches of the lowest order are depicted.

it may become a very significant energy, if the lattice temperature, T , is low in comparison with phonon energy. Then the absorption coefficient should show structures at confined acoustic modes energies. For typical FSQWs, it happens in a terahertz range of frequencies.

Acoustic phonon modes and their spectrum in an isotropic solid slab have been known for a long time [6]. Electron interactions with these acoustic modes through the deformation potential and through the piezoelectric potential were obtained [7]. In a solid slab, there are three types of acoustic modes which differ in their specific symmetry: dilatational, flexural, and shear. As an illustration, the acoustic phonon dispersion relation for ten lowest dilatational modes, calculated for GaAs FSQW of width 100 Å, is shown in Fig. 1.

In this paper, we will employ the quantum kinetic equation for electrons [8–10] in a FSQW placed in a high-frequency electric field and which interact with confined acoustic phonons through the deformation potential. Electron absorption and emission of photons with simultaneous scattering by confined acoustic phonons (which is required to conserve the in-plane wave vector) results in a structure in the absorption coefficient due to scattering by different phonon modes.

2. Absorption Coefficient

We consider FSQW which is situated in the x - y plane with axis z perpendicular to the quantum well. The electromagnetic wave propagates in the z direction, and the electric field of the electromagnetic wave is given by the formula $-E \cos \Omega t$. We use the gauge with zero scalar potential so that the electron Hamiltonian has the form $H_e = \sum_k \varepsilon_k(t) a_k^\dagger a_k$, where $k = (n, \mathbf{k})$, n is electron subband number, \mathbf{k} is electron in-plane wave vector, $\varepsilon_k(t) \equiv \varepsilon_{n,\mathbf{k}}(t) = \varepsilon_n + (\hbar \mathbf{k} + e\mathbf{E}/\Omega \sin \Omega t)^2 / 2m^*$, and m^* is the effective mass.

The acoustic phonon Hamiltonian in FSQW, H_p , has the standard form $H_p = \sum_q \hbar \omega_q b_q^\dagger b_q$, where the quantum number $q = (\alpha, m, \mathbf{q})$ includes the phonon symmetry α (α takes values from the set *dilatational*, *flexural*, *shear*), the mode number m , and the in-plane wave vector \mathbf{q} .

The Hamiltonian for electron interactions with acoustic phonons has the standard form

$$H_{e-p} = \sum_{k,k',q} w(k,k',q) a_k^\dagger a_k b_q + h.c., \quad (1)$$

where *h.c.* stands for Hermitian conjugate terms,

$$w(k,k',q) = \delta_{k',k+q} \langle n' | \Gamma(\alpha, m, q) | n \rangle, \quad (2)$$

$\langle n' | \Gamma(\alpha, m, q) | n \rangle$ is the matrix element between electron subbands *n* and *n'* due to the interaction through acoustic phonon (α, m, q) given in Ref. [7].

The kinetic equation for the diagonal components of the one-electron density matrix, $f_{n,k}(t)$, may be written in the form

$$\frac{\partial f_{n,k}(t)}{\partial t} = J(f|n, k, t), \quad (3)$$

where the collision integral, $J(f|n, k, t)$, is similar to the collision integral considered in Refs. [8–10], except the following two points: (1) the electron states are described by the subband number and electron in-plane wave vector instead by three-dimensional wave vectors; (2) phonons are also described by the mode number and by phonon in-plane wave vector instead of bulk phonon wave vector. The electron distribution defined by eqn (3) is periodic, $f_{n,k}(t) = f_{n,k}(t + 2\pi/\Omega)$, and it may be expanded in the Fourier series

$$f_{n,k}(t) = \sum_v f_{n,k}^{(v)} e^{iv\Omega t}. \quad (4)$$

When the frequency of the electromagnetic field is high compared with the inverse of the average collision time $\bar{\tau}$, $\Omega\bar{\tau} \gg 1$, the first harmonic of the function $f_{n,k}(t)$ is given by the formula

$$f_{n,k}^{(1)} = \frac{1}{2\pi i} \int_{-\pi/\Omega}^{\pi/\Omega} dt \exp(-i\Omega t) J(f^{(0)}|n, k, t). \quad (5)$$

If the electric field intensity is relatively low, so that $eE|q|/m^*\Omega^2 \ll 1$ (i.e. the multiphoton processes are negligible [8]), and if we can neglect the electron heating, then $f_{n,k}^{(0)}$ on the right hand side of eqn (5) can be taken in the form of the equilibrium Fermi function $f\epsilon_{n,k}$.

The power absorbed by the electron-phonon system, Q , may be determined as an average over the period $2\pi/\Omega$ of the instantaneous absorbed power and is equal to $Q = -ReEj^{(1)}$, where $j^{(1)}$ is the first harmonic of the surface electric current density

$$Rej^{(1)} = -\frac{2e\hbar}{m^*A} \sum_{n,k} k f_{n,k}^{(1)}. \quad (6)$$

It is more convenient to deal with a dimensionless relative absorption coefficient, η , than with the absorbed power Q . η is defined as followed: $\eta = Q/\langle P \rangle$, where $\langle P \rangle = c\sqrt{\kappa}E^2/8\pi$ is the Poynting vector averaged over a period, κ is the dielectric constant. From the definition of η and formulae (5) and (6), we obtained the following formula for the absorption coefficient

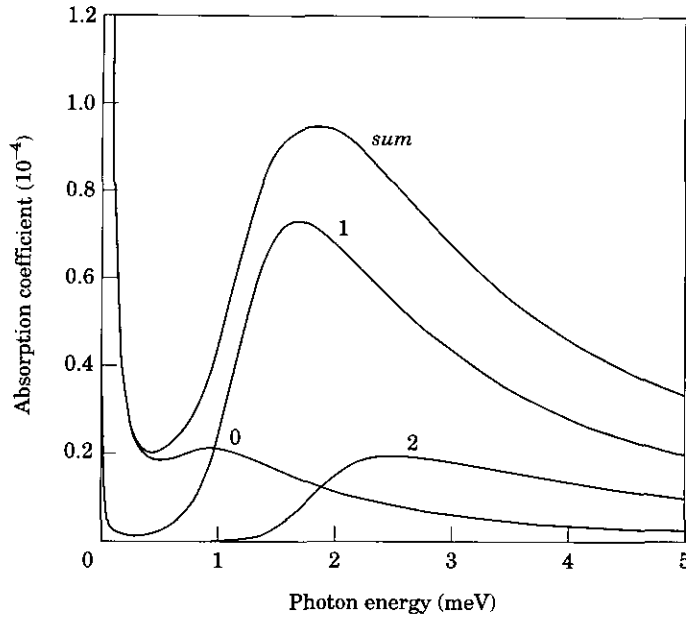


Fig. 2. Absorption coefficient, η , as a function of photon energy (marked as *sum*), and contributions to η due to dilatational modes of order 0, 1, and 2 (curves are marked by the corresponding number). GaAs FSQW of width 10 nm; $\varepsilon_F = 10$ meV.

$$\eta = \frac{e^2}{m^*{}^2 c \Omega^3 \sqrt{\kappa}} \sum_{n,n'} \sum_{\alpha,m,q} \int d\mathbf{k} \mathbf{q}^2 |\langle \pi' | \Gamma(\alpha, m, \mathbf{q}) | n \rangle|^2 \times \{ [(1 - f_{\varepsilon_{n,\mathbf{k}} - \hbar\omega_q + \hbar\Omega}) f_{\varepsilon_{n,\mathbf{k}}} + (f_{\varepsilon_{n,\mathbf{k}}} - f_{\varepsilon_{n,\mathbf{k}} - \hbar\omega_q + \hbar\Omega}) N_q] \times \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{n',\mathbf{k}-\mathbf{q}} - \hbar\omega_q + \hbar\Omega) - [(1 - f_{\varepsilon_{n,\mathbf{k}}}) f_{\varepsilon_{n,\mathbf{k}} + \hbar\omega_q + \hbar\Omega} + (f_{\varepsilon_{n,\mathbf{k}} + \hbar\omega_q + \hbar\Omega} - f_{\varepsilon_{n,\mathbf{k}}}) N_q] \times \delta(\varepsilon_{n,\mathbf{k}} - \varepsilon_{n',\mathbf{k}+\mathbf{q}} + \hbar\omega_q + \hbar\Omega) \}. \quad (7)$$

We have calculated the integral in eqn (7) numerically, employing the acoustic phonon modes and matrix elements for FSQW. We restricted our consideration to the deformation potential interaction of electrons with acoustic phonons, for other mechanisms of scattering give smaller contributions to the interaction.

3. Results

In this paper, we discuss the absorption coefficient for GaAs FSQW. Our calculations have been carried out for FSQW of an intermediate thickness $a = 100$ Å, a low lattice temperature $T \approx 1$ K, and for a surface electron concentration of $n_s = 3 \times 10^{11} \text{ cm}^{-2}$. Under these conditions, only the lowest electron subband is occupied, therefore, $n = n' = 1$ in eqn (7). In addition, due to selection rules related to the symmetry of the phonon modes, only dilatational phonon modes contribute to the electron scattering; therefore, $\alpha = \text{dilatational}$ in eqn (7).

We have calculated the absorption coefficient as a function of photon energy and lattice temperature. Figure 2 demonstrates the dependence of η on the photon energy; the partial absorption coefficients due to phonon modes 0, 1, and 2 are also depicted. The contributions of higher order modes are negligible. Though different phonon modes make their contributions to photon absorption preferentially at different photon energies, the total absorption coefficient does not exhibit the acous-

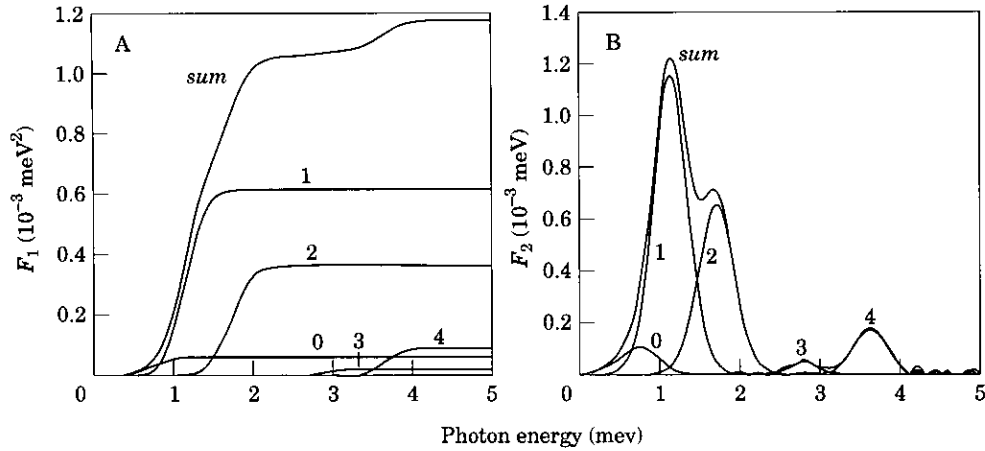


Fig. 3. The first derivative (A) and the second derivative (B) of the function $F_0 = \eta(\hbar\Omega)^3$ with respect to $\hbar\Omega$ as a function of $\hbar\Omega$ (marked by index *sum*). The curves marked 0, 1, 2, 3, 4, and 5 display the contributions of modes 0, 1, 2, 3, 4, and 5, respectively. GaAs FSQW of width 10 nm; $\varepsilon_F = 10$ meV.

tic phonon mode structure. The steep increase of η in the low energy region is due to the factor $1/\Omega^3$, which is not related to specific features of a FSQW and is merely a consequence of the electron gas dielectric function. The strong frequency dependence $1/\Omega^3$ hides the features of the absorption coefficient which are pertinent to a FSQW. For this reason, we introduce a measurable function $F_0 = \eta(\hbar\Omega)^3$, which is related to η .

Characteristic features of the absorption coefficient are much more pronounced in the derivatives of F_0 : $F_1 = dF_0/d(\hbar\Omega)$, $F_2 = dF_1/d(\hbar\Omega)$. Figure 3 demonstrates the first (A) and the second (B) derivatives of F_0 as functions of photon energy (we marked this curve with the index *sum*) as well as the contributions of the modes 0 through 5. The first derivative has clearly pronounced steps and the second derivative has maxima at energies corresponding to the dilatational phonon energies. Small oscillations in the energy range 4–5 meV are due to computational error, the relative significance of which is larger in the region of higher energy where the function is small.

Figure 3 demonstrates that the first dilatational phonon makes the largest contribution to the absorption coefficient. This result agrees with the previous result on the role of the first dilatational mode in limiting the electron mobility [11]. The physical reason for the relative 'weight' of different modes is the spatial distribution of the field of relative displacement in the modes. The zeroth-order mode has a substantial surface-bound character and its overlap with the electron wave function of the first subband is small. The modes of the higher than the first order make too many oscillations across the FSQW width. This results in a decrease of the electron–phonon overlap in comparison to the first mode. However, this dependence on the mode number is not monotonic and depends on the details of the spatial distribution of the relative displacements, as can be seen on Fig. 3(b).

The absorption coefficient is sensitive to the lattice temperature. We calculated the temperature dependence of η for several fixed photon energies. Figure 4 demonstrates the second derivatives of the relative absorption coefficient, $d^2\eta/dT^2$, versus the lattice temperature for $\hbar\Omega = 0.5$ meV (A) and 1.2 meV (B). The contributions of different modes are also shown. The maxima in these derivatives are broad and do not allow an identification of separate modes; however, even in this case, the graphs have structures associated with confined acoustic modes. The steep increase of the second derivative, $d^2\eta/dT^2$, as a function of T in the low temperature region of Fig. 4(B) occurs because the energy of absorbed photon, 1.2 meV, is very close to the cut-off energy for the first dilatational mode, where it has very high density of states. For this reason, the absorption coefficient is very sensitive to a slight change in the lattice temperature.

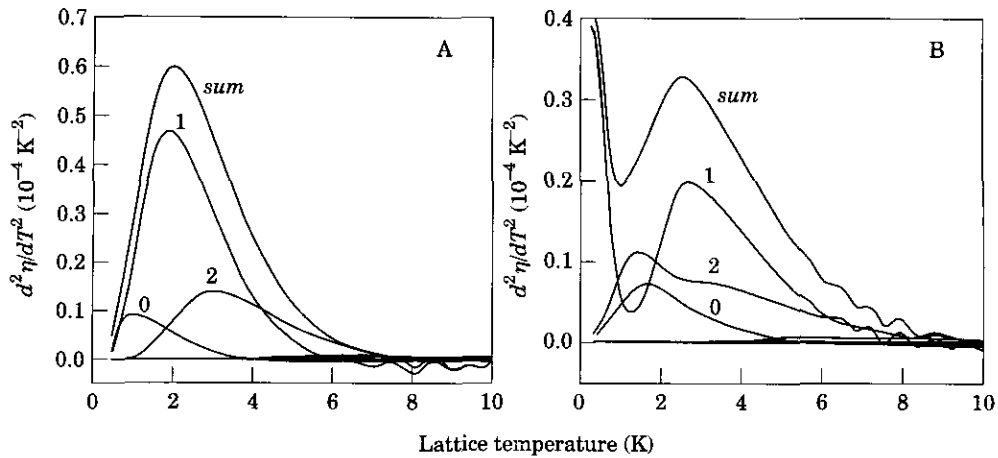


Fig. 4. The second derivative of the relative absorption coefficient with respect to T as a function of lattice temperature for $\hbar\Omega=0.5$ meV (A) and 1.2 meV (B) (the curves marked by index *sum*). The curves marked by indices 0, 1, and 2 correspond to contributions from the zeroth, first, and second dilatational modes. GaAs FSQW of width 10 nm; $\varepsilon_F=10$ meV.

4. Summary

We have demonstrated that the absorption coefficient of an electromagnetic wave in thin solid films carries information about confined acoustic phonons. The positions of the maxima in the frequency dependence of the second derivative of the absorption coefficient multiplied by Ω^3 with respect to Ω correspond to the acoustic phonon energy. The spectral dependencies of the absorption coefficient in the range 0.1–1 THz can be used to identify the confined acoustic phonon modes and to obtain the strength of the electron–phonon interaction. The small absolute value of the absorption coefficient is related to the small surface electron concentration ($3 \times 10^{11} \text{ cm}^{-2}$ in our calculations). Therefore, the modulated spectroscopy techniques are of great importance for the measurements of the discussed spectra. At the same time, the relative absorption coefficient may be several orders of magnitude higher in the case of thin metal films due to a much higher electron concentration.

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