Influence of quantum well parameters on the spectrum of two-dimensional plasmons in HgTe/CdHgTe heterostructures

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Influence of parameters of a quantum well and electronic polarizability spatial dispersion on the dependence of two-dimensional plasmon energy on wave vector in narrow-gap CdHgTe quantum wells (band gap 35 meV) is studied theoretically. It is shown that at energies above 20 meV, the dispersion law of two-dimensional plasmons is close to linear. Taking into account the finite width of the quantum well decreases the plasmon phase velocity. This effect increases with an increase in the fraction of cadmium in the QW while maintaining the band gap and with a decrease in the concentration of charge carriers in it.

Keywords: two-dimensional plasmon, narrow-gap HgTe.

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1. Introduction

It is well known that for the wave vectors $\mathbf{q}$, much greater than ω/c (ω is the frequency, c is speed of light in vacuum), the frequency of the two-dimensional (2D) plasmon is proportional to a square root of its wave vector [1]. However, this dependence is true only when the spatial dispersion of polarizability of the 2D electron gas is not critical [1] (i.e. $\mathbf{q}$ is much smaller than the Fermi wave vector of the electrons). Besides, when finding the dispersion law of the two-dimensional plasmon, it is often assumed that the plasmon wavelength is much bigger than the quantum well width. Usually, these conditions are well observed for the plasmons with the frequencies up to 1 THz in the systems with the GaAs quantum wells [2]. However, both the conditions can be broken when considering interband two-dimensional plasmons, whose energy exceeds the band gap of the HgTe quantum well [3], which somewhat exceed the energy of the longitudinal optical phonon in CdHgTe (21 meV). The interest in these plasmons has arisen in relation to their stimulated lasing in narrow-gap HgTe quantum wells [3]. Note that taking into account the spatial dispersion of polarizability of the electron gas in graphene results in the dependence of the plasmon frequency on its wave vector, which is very different from the root one within the high frequencies [4]. However, if for the graphene plasmons the graphene thickness can be neglected in comparison with the wavelength of the 2D plasmon, then for the HgTe quantum wells the quantum well width is not always small in comparison with the plasmon wave length. In this regard, there is an issue of how the dispersion law for the 2D plasmon will change when taking into account the final width of the quantum well. This issue is important, for example, when calculating a rate of recombination of non-equilibrium carriers with plasmon emission or when calculation a plasmon gain in the conditions of inverse population of the bands.

The present paper is devoted to theoretical study of influence of the spatial dispersion of susceptibility and parameters of the quantum wells, including the width, on the dispersion law of the two-dimensional plasmons in the HgTe/CdHgTe heterostructures with the quantum wells.

2. Method of calculation of the spectrum of the two-dimensional plasmons

In order to find the plasmon dispersion law, we will apply a quasi-static approximation to neglect retardation effects therein [5]. Besides, for simplicity, we will assume that the permittivity κ is the same in the barriers and wells. As we have interest in the plasmons with the frequency bigger than the frequency of the optical phonons, we will assume that the permittivity value is equal to its high-frequency value. Let us assume that a potential wave with the wave vector $\mathbf{q}$ and the frequency ω is propagating along the quantum well:

$$\varphi(\mathbf{r}, t) = \varphi(z)\exp(i\mathbf{qr} - i\omega t + \alpha t) + \varphi^*(z)\exp(-i\mathbf{qr} + i\omega t + \alpha t), \quad (1)$$

where $\alpha > 0$ is an infinitely small value, which is required to correctly go around poles, which appear when calculating the polarizability of the electron gas (see, for example, how the Lienhard formula is obtained in the book [6]). The axis z is selected to be normal to the quantum well. Let us assume that the wave function of the electron in the quantum well with no potential is $\psi^0_{\mathbf{k},s}(z)\exp(i\mathbf{kr})/\sqrt{S}$, where the index s describes both an electron's spin state and a number of

a dimensional quantization subband, S is an area of the quantum well, $\mathbf{r}$ is the radius-vector, $\mathbf{k}$ is the wave vector in the quantum well. The first correction of the perturbation theory to the electron wave function due to the potential (1) is

$$\psi^{(1)}_{\mathbf{k},s}(z,t) = \sum_{s'} b_{s,s'}(\mathbf{k}+\mathbf{q},t)\psi_{\mathbf{k}+\mathbf{q},s'}(z)\exp\big[i(\mathbf{k}+\mathbf{q})\mathbf{r}\big] + c_{s,s'}(\mathbf{k}-\mathbf{q},t)\psi_{\mathbf{k}-\mathbf{q},s'}(z)\exp\big[i(\mathbf{k}-\mathbf{q})\mathbf{r}\big], \quad (2)$$

where

$$b_{s,s'}(\mathbf{k}+\mathbf{q},t) = -e\,\frac{\exp[-i\omega t - i\varepsilon_s(\mathbf{k})t/\hbar + i\varepsilon_{s'}(\mathbf{k}+\mathbf{q})t/\hbar + \alpha t]}{\varepsilon_s(\mathbf{k}) + \hbar\omega - \varepsilon_{s'}(\mathbf{k}+\mathbf{q}) + i\hbar\alpha} \times \int dz\,\psi^*_{\mathbf{k}+\mathbf{q},s'}(z)\varphi(z)\psi_{\mathbf{k},s}(z), \quad (3)$$

$$c_{s,s'}(\mathbf{k}-\mathbf{q}) = -e\,\frac{\exp[i\omega t - i\varepsilon_s(\mathbf{k})t/\hbar + i\varepsilon_{s'}(\mathbf{k}-\mathbf{q})t/\hbar + \alpha t]}{\varepsilon_s(\mathbf{k}) - \hbar\omega - \varepsilon_{s'}(\mathbf{k}-\mathbf{q}) + i\hbar\alpha} \times \int dz\,\psi^*_{\mathbf{k}-\mathbf{q},s'}(z)\varphi^*(z)\psi_{\mathbf{k},s}(z), \quad (4)$$

e is the electron charge, $\varepsilon_s(\mathbf{k})$ is the electron energy with the wave vector $\mathbf{k}$ in the s-th subband, $\hbar$ is the Planck constant. The charge density due to the addition to the wave function (2) is

$$\rho(z,t) = -e\sum_{k,s}\big(|\psi^{(0)}_{\mathbf{k},s}(z,t) + \psi^{(1)}_{\mathbf{k},s}(z,t)|^{(2)} - |\psi^{(0)}_{\mathbf{k},s}(z,t)|^{(2)}\big) f_s(\mathbf{k}), \quad (5)$$

where $f_s(\mathbf{k})$ is the function of distribution of the electrons in the s--th subband. Using the equations (2)–(4), the expression (5) can be represented as follows

$$\rho(z,t) = e^2\sum_{\mathbf{k},s,s'}\psi^*_{\mathbf{k},s}(z)\psi_{\mathbf{k}+\mathbf{q},s'}(z) \times \frac{\exp(i\mathbf{qr}-i\omega t)f_s(\mathbf{k})}{\varepsilon_s(\mathbf{k}) + \hbar\omega - \varepsilon_{s'}(\mathbf{k}+\mathbf{q}) + i\hbar\alpha} \times \int dz\,\psi^*_{\mathbf{k},s'}(z)\varphi(z)\psi_{\mathbf{k},s}(z) - e^2\sum_{\mathbf{k},s,s'}\psi^*_{\mathbf{k}-\mathbf{q},s'}(z)\psi_{\mathbf{k}+\mathbf{q},s'}(z) \times \frac{\exp(i\mathbf{qr}-i\omega t)f_s(\mathbf{k})}{\varepsilon_s(\mathbf{k}) - \hbar\omega - \varepsilon_{s'}(\mathbf{k}-\mathbf{q}) - i\hbar\alpha} \times \int dz\,\psi_{\mathbf{k}-\mathbf{q},s'}(z)\varphi(z)\psi^*_{\mathbf{k},s}(z) + c.c., \quad (6)$$

where the symbol $c.c.$ signifies a complex conjugate summand.

It is clear from the formula (6) that the charge density can be divided into two parts corresponding to $\varphi(z)$ and $\varphi^*(z)$, which can be separately considered. For that reason, in the potential (1) and the charge density (6) we will further consider the those summands which are proportional to $\varphi(z)$. Let us re-write the formula (6) more conveniently:

$$\rho(\mathbf{r}) = \frac{e^2\exp(i\mathbf{qr}-i\omega t)}{S} \times \sum_{\mathbf{k},s,s'}\frac{\psi^*_{\mathbf{k},s}(z)\psi_{\mathbf{k}+\mathbf{q},s'}(z)\big(f_s(\mathbf{k}) - f_{s'}(\mathbf{k}+\mathbf{q})\big)}{\varepsilon_s(\mathbf{k}) + \hbar\omega - \varepsilon_{s'}(\mathbf{k}+\mathbf{q}) + i\hbar\alpha} \times \int dz'\psi^*_{\mathbf{k}+\mathbf{q},s'}(z')\varphi(z')\psi_{\mathbf{k},s}(z'). \quad (7)$$

Using (7), the Poisson's equation can be represented as

$$-q^2\varphi(z) + \frac{d^2}{dz^2}\varphi(z) = -\frac{4\pi}{\kappa}\,\frac{e^2\exp(i\mathbf{qr}-i\omega t)}{S} \times \sum_{\mathbf{k},s,s'}\frac{\psi^*_{\mathbf{k},s}(z)\psi_{\mathbf{k}+\mathbf{q},s'}(z)\big(f_s(\mathbf{k}) - f_{s'}(\mathbf{k}+\mathbf{q})\big)}{\varepsilon_s(\mathbf{k}) + \hbar\omega - \varepsilon_{s'}(\mathbf{k}+\mathbf{q}) + i\hbar\alpha} \times \int dz'\psi^*_{\mathbf{k}+\mathbf{q},s'}(z')\varphi(z')\psi_{\mathbf{k},s}(z'), \quad (8)$$

where $q = |\mathbf{q}|$.

Using the Fourier transformation for the function $\varphi(z)$, the integro-differential equation (8) can be transformed into the integral equation:

$$\varphi(z) = \frac{4\pi e^2}{\kappa S}\int dk_z\exp(ik_z z)\sum_{\mathbf{k},s,s'}\frac{g_{s,s'}(\mathbf{k},\mathbf{k}+\mathbf{q},k_z)}{(q^2+k_z^2)} \times \frac{\big(f_s(\mathbf{k}) - f_{s'}(\mathbf{k}+\mathbf{q})\big)}{\varepsilon_s(\mathbf{k}) + \hbar\omega - \varepsilon_{s'}(\mathbf{k}+\mathbf{q}) + i\hbar\alpha} \times \int dz'\psi^*_{\mathbf{k}+\mathbf{q},s'}(z')\varphi(z')\psi_{\mathbf{k},s}(z'), \quad (9)$$

where

$$g_{s,s'}(\mathbf{k},\mathbf{k}+\mathbf{q},k_z) = \int dz\exp(-ik_z z) \times \psi^*_{\mathbf{k},s}(z)\psi_{\mathbf{k}+\mathbf{q},s'}(z)(2\pi)^{-1/2}.$$

In order to find the solutions (9), we will make two simplifying assumptions. The first one is that we will neglect the dependence $\int dz'\psi^*_{\mathbf{k}+\mathbf{q},s'}(z')\varphi(z')\psi_{\mathbf{k},s}(z')$ on $\mathbf{k}$, $\mathbf{q}$, and we will also assume that this integral is non-zero only for $s = s'$, wherein the integral does not depend on the electron spin in each dimensional quantization subband. Note that this assumption is accurate when the electron movements along and across the quantum well are mutually independent. The numerical analysis of the functions for $\psi^*_{\mathbf{k}+\mathbf{q},s'}(z')\psi_{\mathbf{k},s}(z')$ of the two quantum wells to be discussed below, in which $dq \le 1$ (d is the QW width), shows the adequacy of these approximations.

Using this assumption, indices corresponding to the wave vector in the integral $\int dz'\psi^*_{\mathbf{k}+\mathbf{q},s'}(z')\varphi(z')\psi_{\mathbf{k},s}(z')$, can be omitted.

The second assumption is that the spectrum is degenerate in terms of a spin and the electrons fill only the lower dimensional quantization subband in the conductivity band and the holes are only in the highest valence subband. That is why instead of s we will use the index c for the conductivity band and the index v for the valence band. Multiplying (9) first by $\psi_c^*(z)\psi_c(z)$ and integrating by z, and then making a similar operation with the wave functions of the valence band, we obtain the system of the two equations:

$$I_c = I_c \int dk_z \frac{g_{c,c}(k_z) g_{v,v}(-k_z)}{q^2 + k_z^2} A_c(q, \omega) + I_v \int dk_z \frac{g_{v,v}(k_z) g_{c,c}(-k_z)}{q^2 + k_z^2} A_v(q, \omega)$$

$$I_v = I_c \int dk_z \frac{g_{c,c}(k_z) g_{v,v}(-k_z)}{q^2 + k_z^2} A_c(q, \omega) + I_v \int dk_z \frac{g_{v,v}(k_z) g_{v,v}(-k_z)}{q^2 + k_z^2} A_v(q, \omega), \qquad (10)$$

where

$$I_j = \int dz' \varphi(z') \psi_j^*(z') \psi_j(z')$$

$$A_j(q, \omega) = \frac{2e^2}{\kappa\pi} \int d^2k \frac{\left(f_j(\mathbf{k}) - f_j(\mathbf{k}+\mathbf{q})\right)}{\varepsilon_j(\mathbf{k}) + \hbar\omega - \varepsilon_j(\mathbf{k}+\mathbf{q}) + i\hbar\alpha}, \qquad (11)$$

where $j = c, v$.

As (10) is a system of two linear homogeneous equations in relation to I_c and I_v, a condition of existence of the non-trivial solution is the fulfillment of the equality as follows:

$$\left[\int dk_z \frac{g_{c,c}(k_z) g_{c,c}(-k_z)}{q^2 + k_z^2} A_c(q, \omega) - 1\right] \times \left[\int dk_z \frac{g_{v,v}(k_z) g_{v,v}(-k_z)}{q^2 + k_z^2} A_v(q, \omega) - 1\right] - \int dk_z \frac{g_{v,v}(k_z) g_{c,c}(-k_z)}{q^2 + k_z^2} A_v(q, \omega) \times \int dk_z \frac{g_{c,c}(k_z) g_{v,v}(-k_z)}{q^2 + k_z^2} A_c(q, \omega) = 0, \qquad (12)$$

which is an equation for finding the dependence of the plasmon frequency on its wave vector. When the localization size of the wave functions along the z axis is much smaller than $1/q$, the following relationships are true

$$g_c(k_z) = g_v(k_z) = (2\pi)^{-1/2},$$

$$\int dk_z \frac{g_c(k_z) g_c(-k_z)}{q^2 + k_z^2} = \frac{1}{2q}. \qquad (13)$$

Then (12) can be represented as follows

$$1 = \frac{2\pi e^2}{q\kappa S} \sum_k \left[\frac{f_c(\mathbf{k}) - f_c(\mathbf{k}+\mathbf{q})}{\varepsilon_c(\mathbf{k}) + \hbar\omega - \varepsilon_c(\mathbf{k}+\mathbf{q}) + i\hbar\alpha} + \frac{f_v(\mathbf{k}) - f_v(\mathbf{k}+\mathbf{q})}{\varepsilon_v(\mathbf{k}) + \hbar\omega - \varepsilon_v(\mathbf{k}+\mathbf{q}) + i\hbar\alpha}\right], \qquad (14)$$

which corresponds to „usual“ (i.e. when the quantum well width is assumed to be infinitely small) the dispersion equation for the plasmons with taking into account the spatial dispersion of the polarizability of the electron and hole gas [1]. Thus, we have demonstrated that in the limit case (12) converts to the „usual“ equation for finding the dispersion law of the two-dimensional plasmon, which takes into account the spatial dispersion of polarizability of the electron gas.

3. Results and discussion

The calculation has been performed for the structures grown on the (013) CdTe plane, as they are the most frequently used for observing the lasing [7–9]. The concentrations of the electrons and holes have been assumed to be the same, so has the temperature $T = 4.2$ K. The functions of electron distribution in the bands have been assumed to be equal to

$$f_j(\mathbf{k}) = \left[1 + \exp\left(\frac{\varepsilon_j(\mathbf{k}) - F_j}{k_B T}\right)\right]^{-1}, \qquad (15)$$

where k_B is the Boltzmann's constant. The values of the chemical potentials in the bands have been found from the condition of equality of the concentrations of the electrons and the holes, which are calculated by means of (15) to the given concentrations.

For calculation of the electron states, the Kane model has been used taking into account deformation effects. For simplicity, we have neglected a reduced symmetry of the structure on heterointerfaces and no inversion center, thereby resulting in two-fold degeneration of the electron spectrum. The calculation details can be found in [10]. The two quantum wells with the same band gap (35 meV) have been considered, but they had different widths: 5 and 11.75 nm and were surrounded by the $Cd_{0.7}Hg_{0.3}Te$ barriers. A material for the 5 nm — quantum well has been assumed to be HgTe, so for 11.75 nm — quantum well has $Cd_{0.1}Hg_{0.9}Te$. Fig. 1 shows the electron spectra for these wells.

Fig. 2 shows the calculated dependences of the energy of the two-dimensional plasmon on its wave vector for the HgTe 5 nm quantum well at the two concentrations of the non-equilibrium carriers $n = p = 2 \cdot 10^{11}$ and $5 \cdot 10^{11}$ cm^{-2}. The solid curves are obtained by solving the equation (12), so are the dotted by solving the equation (14). It is clear from Fig. 2 that for the energies of the plasmon

> 20 meV the dependence of the plasmon frequency on the wave vector is close to linear $\omega \propto q$. With increase in the concentration of the carriers, the plasmon phase velocity is increasing. Taking into account the finite width of the quantum well decreases the plasmon phase velocity. This effect is more pronounced for lesser concentrations of the carriers. It is clear from Fig. 2 that taking into account the non-zero width of the quantum well in the calculations is similar to effective decrease in the concentration of the carriers in the quantum well.

In order to explain the dependence of the plasmon energy on the wave vector at high values of q, we note that for the big electron wave vectors the dispersion law for the electrons in the conductivity band is close to linear (see Fig. 1), i.e. at the big wave vectors the dependence of the electron energy on the wave vector k can be presented

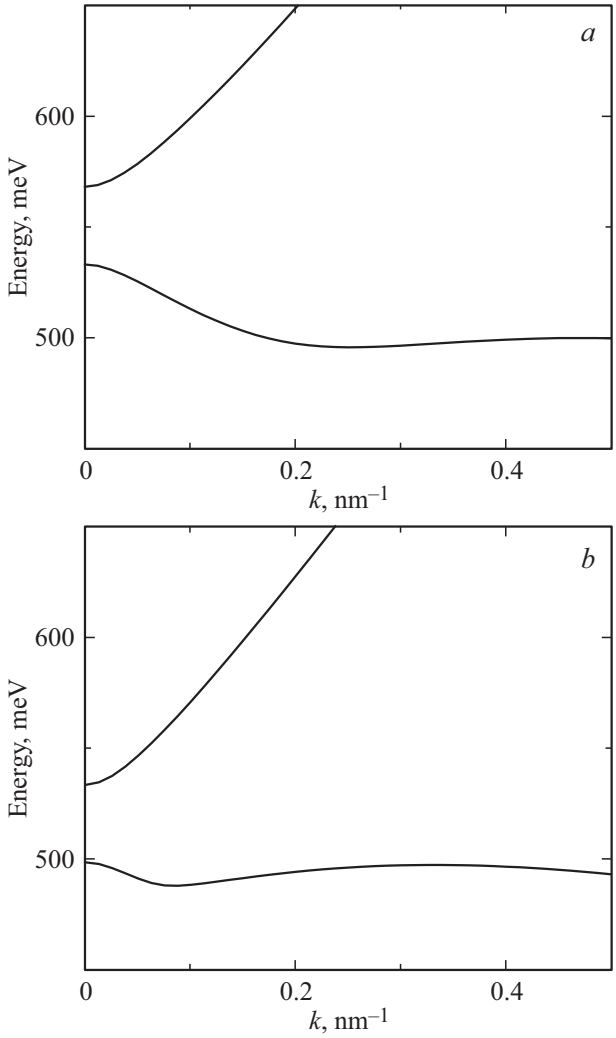

Figure 1. Spectra of the electrons in the quantum wells HgTe with thickness 5 nm (a) and $Cd_{0.1}Hg_{0.9}Te$ with thickness 11.75 nm (b). The wave vector is directed along the [100] crystallographic direction. The quantum wells are grown on the (013) CdTe plane and surrounded by the $Cd_{0.7}Hg_{0.3}Te$ barriers. The temperature is 4.2 K.

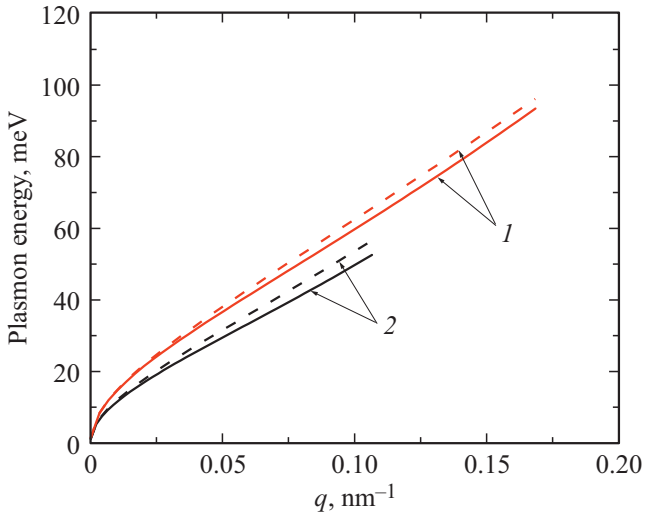

Figure 2. Dependences of the plasmon energy on the wave vector in the HgTe 5 nm — quantum well. The concentrations of the electrons and the holes, cm^{-2}: *1* — $5 \cdot 10^{11}$, *2* — $2 \cdot 10^{11}$ cm^{-2}. The solid lines are resulted from solving the equation (12), so are the dotted — (14).

as $\varepsilon_c(\mathbf{k}) \approx \hbar V k + \varepsilon_0$, where V is the maximum velocity of the electron. Besides, it is clear from Fig. 1 that for the big wave vectors k the effective mass of the holes is much bigger than the mass of the electrons. That is why the hole polarizability is much less than the electron one. For that reason, the dispersion law of the plasmons is mainly determined by the electrons and the second summand in the right part of (14) can be neglected. If $q \gg k_F$, where k_F is the wave vector at the Fermi level, then the right part of (14) can be represented as

$$\frac{2\pi e^2}{q\kappa S} \sum_k \left[\frac{f_c(\mathbf{k}) - f_c(\mathbf{k}+\mathbf{q})}{\varepsilon_c(\mathbf{k}) + \hbar\omega - \varepsilon_c(\mathbf{k}+\mathbf{q}) + i\hbar\alpha} \right]$$

$$\approx \frac{2\pi e^2 n}{\kappa} \frac{\hbar V}{(\hbar\omega)^2 - (\hbar V q)^2}, \qquad (16)$$

where n is the concentration of the electrons in the quantum well. Substituting (16) in (14), we obtain

$$\hbar\omega \approx \sqrt{(\hbar V q)^2 + \frac{2\pi e^2 n \hbar V}{\kappa}}. \qquad (17)$$

It is clear from (17) that with the high q the plasmon frequency linearly depends on the wave vector $\omega \sim q$, while the plasmon group velocity tends to the maximum velocity of the electron. Note that the calculations of the graphene spectrum provide the similar picture [4].

Fig. 3 shows the calculated dependences of the energy of the two-dimensional plasmon on its wave vector for the $Cd_{0.1}Hg_{0.9}Te$ 11.75 nm — quantum well, which is surrounded by the $Cd_{0.7}Hg_{0.3}Te$ barriers. This well has the same band gap as the 5 nm-HgTe quantum well — 5 nm. Adding cadmium to the quantum well increases its

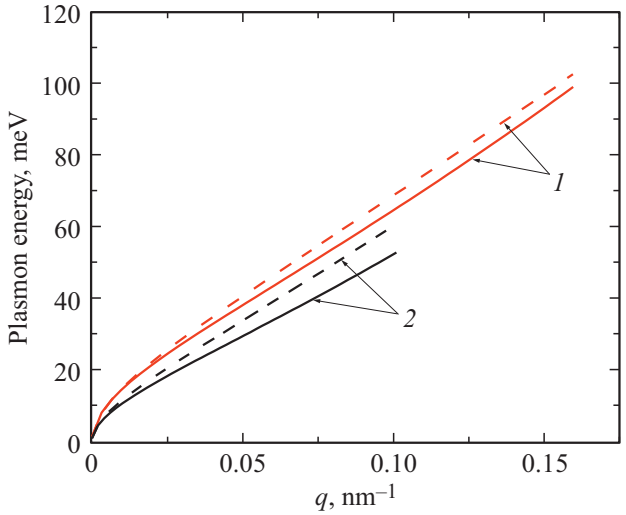

Figure 3. Dependence of the plasmon energy on the wave vector in the $Cd_{0.1}Hg_{0.9}Te$ 11.75 nm — quantum well. The concentrations of the electrons and the holes, cm^{-2}: *1* — $5 \cdot 10^{11}$, *2* — $2 \cdot 10^{11}\,cm^{-2}$. The solid lines are resulted from solving the equation (12), so are the dotted — (14).

thickness provided that the band gap is maintained. That is why in this situation taking into account the quantum well width when calculating the dispersion law more strongly affects the dependence of the plasmon energy on the wave vector. It is clear from comparison of the figures 2 and 3 that the addition of cadmium slightly increases the plasmon velocity provided that the band gap is maintained. It is also clear from Fig. 3 that for the concentration of the electrons and the holes $2 \cdot 10^{11}\,cm^{-2}$, decrease in the plasmon energy (due to taking into account the QW finite width) is approximately two times bigger than for the concentration $5 \cdot 10^{11}\,cm^{-2}$ at the definite wave vector at a linear section of the dispersion curve.

4. Conclusion

In the conclusion the main results of the study are described. It is shown that at the big vectors of the two-dimensional plasmon the frequency dispersion of polarizability of the current carriers in the quantum well results in the dependence $\omega \propto q$. The group velocity of the plasmons with the big q tends to the maximum velocity of the electron in the lower subband of the dimensional quantization subband. At the given wave vector, taking into account the quantum well width when calculating the dispersion law results in reduction of the plasmon energy like in reduction of the plasmon energy which occurs when reducing the concentration of the charged carriers in the quantum well.

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Conflict of interest

The authors declare that they have no conflict of interest.

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