Plasmon-phonon coupling in lead salt semiconductor quantum well

K H Aharonyan and N B Margaryan
National Polytechnic University of Armenia, 105 Teryan Street, Yerevan 375009, Armenia
ahkamo@yahoo.com

Abstract. The dispersion spectrum peculiarities of intrasubband plasmon-phonon modes applied to realistic narrow-gap EuS / PbS / EuS quantum well are investigated depending on the interplay between the system key parameters, such as quantum well thickness and electron gas density. As follows, the strong mode coupling takes place already for typical moderate 2D densities due to the dielectric confinement effect. The strong dependence of the phonon-like coupled mode damping on the QW width is received in contrast to the plasmon-like mode. The numerical results for the energy-loss function and the oscillator strength of the plasmon-like and phonon-like peaks are also presented. It is shown that in the long wavelength limit a plasmon-like coupled mode contribution in this realistic structure is deeply suppressed and the actual oscillator strength on the whole is connected with the phonon-like part.

The electron-phonon coupling is the macroscopic coupling of the charge-density oscillations (plasmons) of the electron gas (EG) to the lattice longitudinal optical (LO) excitations (LO-phonons). This phenomenon hybridizes the collective plasmons with the LO-phonon modes and gives rise to the coupled plasmon-phonon modes. They have been extensively studied both experimentally and theoretically in bulk and quasi-two-dimensional (Q2D) electron systems, influenced by Q2D spatial confinement and by quantum structure constituent material features [1-13]. The investigations in this field mainly are based on Si, InN, GaAs, III-V group other semiconductors and also on the graphen [14-17]. In most of discussions the media dielectric constant contrast in heteroboundary (dielectric confinement (DC) effect) of QW and barrier is fully ignored.

The lead salt compounds of narrow-gap IV-VI series semiconductors are quite polar semiconductors both with Fröhlich coupling constant of the order of 0.2 ÷ 0.3 and with distinguish DC effect matched possibility due to high value dielectric constants (~10-100). This weak-coupling limit is fairly appropriate and if one can match the momentum and energy of the plasmon and the phonon excitations. So the electric field created by phonons will have a large response due to plasmons.

In this connection, in realistic strongly DC effect matched EuS / PbS / EuS QW nanostructure the dispersion of unretarded Q2D EG intraband plasmons [18] and plasmon-phonons [11-13] are studied theoretically recently. The obtained strong enhancement of plasma, plasmon-like and phonon-like plasmon-phonon modes for moderate low 2D densities (~10^{11} cm^{-2}) attributed to QW/barrier dielectric constants apparent contrast.
Specifically, in the lead salts, the optical LO- and TO- phonon energy difference $\hbar \omega_{LO} - \hbar \omega_{TO}$ in the long wave limit exceeds much more $\hbar \omega_{TO}$ . For example, in the PbS material it exceeds about three times $\hbar \omega_{TO}$ value ($\hbar \omega_{LO} \approx 27.6$ meV, $\hbar \omega_{TO} \approx 8.5$ meV). Thus, the collective elementary plasmon-phonon excitations of EG in the system under discussion are influenced not only by the DC effect and structural features of the QW system, but also the specifics of the optical phonon spectrum of the lead salt semiconductor. At the same time, lead salts have strong nonparabolic bands which must be affecting plasmon-phonon mode corrections. A reasonable measure of the nonparabolicity effects on plasmon-phonon corrections in these systems is $\hbar \omega_{LO} / E_g$, which for PbS material is $\approx 0.09$ (for InSb and GaAs materials it is $\approx 0.1$ and $\approx 0.02$ respectively.

In this paper, the intrasubband plasmon-phonon modes dispersion spectrum peculiarities depending on the interplay between the values of the QW thickness $d$ and 2D EG density $n$, in narrow-gap EuS/PbS/EuS quantum well are presented. The numerical results for the energy-loss function and the oscillator strength of the given plasmon-like and phonon-like peaks are offered as well.

The collective plasmon-phonon modes are given by zeros of the complex total dielectric function

$$
\varepsilon_{Q2D}^{fin} = 1 - \frac{4 \pi e^2}{\varepsilon_w k} F(k) \gamma + \frac{\varepsilon_\infty^0 / \varepsilon_w^0 - \omega^2 / \omega_{LO}^2}{\varepsilon_\infty^0 / \varepsilon_w^0 - \omega^2 / \omega_{LO}^2} = 0, \quad (1)
$$

where $k$ is the 2D wave vector, $F(k) = 2/(kd + 2/\varepsilon_r)$ is the DC influenced Q2D form factor [11].

In the most easily achieved experimentally long-wavelength region ($kd << 1$), where noninteracting polarizability has the form $\gamma = n k^2 / m_w \alpha^2 [2-5]$, the coupled $\omega_-$ and $\omega_+$ unretarded plasmon-like and phonon-like collective modes are characterized by [11]

$$
\omega_- = \frac{\omega_{TO}}{\omega_{LO}} \left[ \frac{4 \pi n_s e^2}{\varepsilon_w^0 m_w} \right]^{1/2} \left[ \frac{k}{kd + (2/\varepsilon_r)} \right]^{1/2}, \quad (2)
$$

and

$$
\omega_+ = \omega_{LO} + \frac{\omega_{TO}^2 - \omega_{LO}^2}{2 \omega_{LO}^2} \left[ \frac{4 \pi n_s e^2}{\varepsilon_w^0 m_w} \right] \left[ \frac{k}{kd + (2/\varepsilon_r)} \right], \quad (3)
$$

where $\varepsilon_r = \varepsilon_\infty^0 / \varepsilon_w^0 \gg 1$. $\varepsilon_\infty^0$, $\varepsilon_w^0$, $\varepsilon_b^\infty$ are the QW and barrier high and low dielectric constants.

Equation (2) shows, that $\omega_-$ plasmon-like mode repeats root square 2D plasmon result [3-5] under very small in-plane vectors $k$ only and is less than the uncoupled 2D plasmon mode due to the factor $\omega_{TO} / \omega_{LO}$. For the PbS sample this reduction is about 70% (i.e. $\omega_{TO} / \omega_{LO} \approx 0.3$) and plasmon-like coupled mode is deeply suppressed. Besides that, $\omega_-$ depends on the barrier dielectric constant $\varepsilon_b$ only and will be strongly enhanced because of its small value. On the other hand, the phonon-like collective mode $\omega_+$ repeats a 2D plasmon-phonon linear result for the DC effect absent case [2, 5] under very small 2D vector $k$ only. For the PbS semiconductor this mode weakly depends on the optical frequency $\omega_{TO}$ because of the specific condition $\omega_+^2 >> \omega_+^2$.

The numerical calculation of plasmon-phonon collective modes in DC effect matched EuS/PbS/EuS QW for moderate low $3.5 \times 10^{11}$ cm$^{-2}$ density case with two different QW width values $d=2.5$ nm and 10 nm carried out. We have chosen the following material and structural parameters in this paper such as: $\varepsilon_0^0 = 170$, $\varepsilon_w^\infty = 17$, $\varepsilon_b^\infty = 5$, $m_w = 0.1 m_0$ and $m_b \approx m_0$. For
$n_s = 3.5 \times 10^{11}$ cm$^2$ the Fermi wave vector is $k_F = 1.5 \times 10^6$ cm$^{-1}$ and the unit of frequency is $2E_F/h = 3.2 \times 10^{13}$ Hz.

Figure 1. The plasma-phonon collective modes in relation to the e-h edges as a function of the wave vector. $\omega_{pl}$ and $k$ are in units of $2E_F/h$ and $k_F$, respectively.

Figure 1 show the collective excitation dispersion curves of the coupled intrasubband plasmon-phonons in relation to e-h excitation continuum (where the unretarded modes are Landau damped) for arbitrary values of the 2D wave vector. The PbS bulk LO- and TO - phonon dispersionless modes are shown as straight lines at points $\omega_{L} = 1.375$ and $\omega_{T} = 0.425$. The plasmon unperturbed mode $\omega_{pl}(k)$ is given as well. Collective excitation dispersion dependences $\omega_{pl}(k)$ are plotted taking into account the condition $\omega_{pl} > \omega_{e-h}$ and the edges of the Landau region $\omega_{e-h}(k) = (2E_F/h) [(k/k_F) + (k^2/2k_F^2)]$.

As follows, the plasmon-phonon collective modes are strongly resolved in relation to the e-h edges and the LO-phonon mode line already at very small wave vectors. Thus, the mode coupling takes place already for typical moderate 2D densities due to the DC effect. This is confirmed by comparing the behaviors of the unperturbed plasmon mode curves in figure 1 (a) and (b) entering the continuum at $(\omega, k) = (1.401, 0.95)$ and $(2.194, 1.32)$ in the cases of $d = 10$ nm to $d = 2.5$ nm, respectively. In both cases the plasmon-like branches are effectively suppressed due to the small material value of the frequency $\omega_{TO}$ and intersects with the continuum at $(\omega, k) = (0.339, 0.295)$ and $(0.362, 0.313)$. By decreasing of the QW width value from $d = 10$ nm to $d = 2.5$ nm, the allowed frequency region of the plasmon-like mode enhances about 7% and remains to be distinguished in the long wave region. In turn, the phonon-like branches are situated effectively higher than LO - phonon mode line $(\omega_{L} = 1.38)$. The spectral curve $\omega_{c-h}$ for the case of $d = 10$ nm ends at the $(\omega, k) = (2.4, 1.41)$ and for the case of
d = 2.5 nm enters the continuum at the \((\omega, k) = (3.61, 1.87)\). As it follows, by decreasing the QW width value from \(d = 10\) nm to \(d = 2.5\) nm the allowed frequency region of the phonon-like mode enhances about 50\% and provides a strong phonon-like coupling in compare to the plasmon-like case. The latter is connected with the suppression of plasmon-like mode in the structure discussed in accordance with figure 1.

The relative importance of different collective excitations becomes apparent if one discuss the dynamical structure factor \(S(\omega, k)\), giving a spectral weight of the collective modes and is proportional to the imaginary part of the inverse dielectric function (energy-loss function). The latter is given by

\[
-\text{Im}[\varepsilon(k, \omega)]^{-1} = \frac{\varepsilon_1}{\varepsilon_1^2 + \varepsilon_2^2},
\]

where \(\varepsilon_1 = \text{Re} \varepsilon(k, \omega), \varepsilon_2 = \text{Im} \varepsilon(k, \omega)\).

For a true collective mode with zero Landau damping both \(\text{Im} \varepsilon(k, \omega)\) and \(\text{Re} \varepsilon(k, \omega)\) vanish, and the inverse dielectric function with spectral weight (oscillator strength)

\[
W(k) = \frac{\pi}{\frac{\partial^2}{\partial \omega^2} \text{Re} \varepsilon(k, \omega)|_{\omega_j(k)}},
\]

where \(\omega = \omega_j(k)\) is the collective mode frequency at wave vector \(k\).

In figure 3 (a) and (b) the calculated energy-loss function \(-\text{Im}[\varepsilon(k, \omega)]^{-1}\) is shown as a function of the mode frequency in the moderate low 2D density case \(n_s = 3.5 \times 10^{11} \text{ cm}^{-2}\), for the different values of the 2D wave vector \(k / k_F = 0.2\) and \(k / k_F = 1\), respectively. The collective modes in the energy-loss spectrum are indicated by vertical arrows and the numbers on the peaks indicate the strength of the collective modes. As follows, for long wave related vector values \((k / k_F = 0.2)\) both the plasmon-like and phonon-like parts are present, but the actual oscillator strength on the whole is connected with the phonon-like part, because the spectral weights are such as: \(W = 0.0052\) and \(W = 1.88\) in the case of \(d = 10\) nm and \(W = 0.0057\) and \(W = 1.84\) for the \(d = 2.5\) nm, respectively.

Actually, in the long wavelength limit the spectral weight of plasmon-like mode almost vanishes, but the weight of phonon-like mode is finite and has most of the weight. Thus, in the long wavelength limit, the whole all spectral weight is carried by the phonon-like mode. Mainly this is a consequence of small material value of the frequency \(\omega_{\text{TO}}\), for that the plasmon-like mode quickly merges with the electron-hole continuum at a critical wave vector, which is much smaller than that of the uncoupled mode critical wave vector (marked by a cross on the \(\omega_{\text{e-h}}\) curve). For large wave vectors \((k / k_F = 1)\), the plasmon-like part is absent and spectral weights of phonon-like modes are \(W = 1.88\) in the case of \(d = 10\) nm and \(W = 1.84\) for the \(d = 2.5\) nm, respectively. As follows, in the last case the oscillator strength is transferred to the phonon-like peak and to the pair-excitation continuum. Besides, by decreasing of the QW width, the spectral weight of phonon-like modes for the long wave related vector case decreases weakly (2\%). In turn, for large wave vector case \((k / k_F = 1)\) the spectral weight, on the contrary, increases noticeably (17.5\%). Thus, in narrow QW, the plasmon-phonon coupling goes strong for the phonon-like modes only. The latter is consistent with the results in figure 1 (b), where both uncoupled and coupled excitation curves are enhanced in relation to LO- and TO-phonon dispersionless curves.
Figure 2. The energy-loss function as a function of frequency for the wave vector values of $k = 0.2$ and 1.1 respectively. The arrows indicate the collective modes. $k$ and $\omega_{pl-phon}$ are in units of $k_F$ and $2E_F/h$.

In summary, we have calculated the dispersion and the spectral weight of the coupled plasmon-phonon modes in realistic dielectric confinement effect matched narrow-gap EuS / PbS / EuS QW structure depending on the interplay between the QW thickness and Q2D EG density. We find that by decreasing the QW width for typical moderate low 2D densities ($3.5 \times 10^{11} \text{cm}^{-2}$) the effect provides a strong phonon-like coupling in compare to the plasmon-like case, which is connected with the constituent material features of the structure discussed.

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