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PLASMON MODE FEATURES IN PbSe-BASED FREE-STANDING SEMICONDUCTOR QUANTUM WIRES

The features of the dispersion spectrum of quasi-dimensional plasmon modes in free-standing PbSe based quantum wires in the presence of strong dielectric mismatch are discussed. It is shown that in such a nanosystem, in addition to plasmonic intraband oscillations at the long wave limit, alternative long wave related oscillations can occur, the frequency of which does not depend on the wave vector and simultaneously increases with decreasing the wire thickness. The numerical analysis of the allowed plasmon spectral characteristic range is performed.

Keywords: free-standing quantum wire, plasmon, dispersion spectrum.

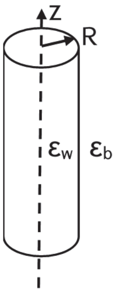
1.Introduction. At present, an inclusive interest of quasi-one-dimensional electron gas (Q1D EG) properties in semiconductor quantum wires (QWr), nanorods, nano-whiskers or carbon nanotubes is initiated by applying the potential of these structures in high-speed electronic and optical devices. An advanced selective doping makes it possible to spatially separate free carriers in Q1D EG from the parent ionized impurities and investigate the charged Q1D system rather than the neutral electron-hole plasma [1].

A realistic semiconductor QWr can either be free-standing or surrounded with a barrier environment appropriate to the device application. In this sense, for the charge carrier Q1D system - based devices, the use of the low dielectric constant barrier environment (lower than the semiconductor QWr dielectric constant) is favorable [2]: a) as it enhances the Coulomb interaction between the charges inside the QWr (dielectric confinement effect (DC)), b) leads to the new features that are absent in the dielectrically homogeneous QWr system [1].

Such tunability of the Coulomb interaction in the QWr modifies many body effects, in particular, the collective plasmon excitations of the Q1D EG. As shown in [3], the DC affected Q1D intrasubband plasmon modes for a long wave limit are independent of the dielectric screening of the QWr and is wholly screened by the surrounding barrier environment as in the Q2D intrasubband case in quantum wells (QW) [4]. In turn, as obtained by Aharonyan et al [5], in the presence of a strong DC effect, there exists a distinct q 1D wave vector ranging in the long wave limit that the corresponding collective plasmon modes are characterized by qualitatively different dispersion analytical laws. In particular, with the result obtained before[3], there exist as well moderately long wave-related vectors for those Q1D intrasubband plasmon modes analogous with the 3D bulk plasmons independent of

q and increase with decreasing the QWr thickness (radius) as for the QW [4] and supperlattice cases [6].

At the same time, a proper realistic model, corresponding to such types of collective modes is not presented in [5] and has really been done in this article. This work presents the Q1D EG dispersion spectrum features of the nonretarded collective plasmon modes in realistic PbSe-based free - standing semiconductor QWr in the presence of a strong DC effect.



2.Theory. Let us now consider an infinitely long semiconductor cylindrical QWr of a radius R filled with an active material with the dielectric constant ε_w, immersed in a dielectric barrier environment with the dielectric constant ε_b and contains free electrons distributed with an average linear concentration N_l.

The polar coordinates (ρ, φ, z) are elaborated here and let the z axis coincide with the QWr axis . The electron motion parallel to the QWr axis is considered freely in the effective mass approximation and for simplicity, the electron effective mass tensor is taken to be diagonal with $m_x = m_y = m_t$, $m_z = m_l$. The motion perpendicular to the QWr axis is quantized and the model of a square well with infinite walls is adopted.

It is assumed that the electron plasma is weakly nonideal, i.e. the effect of the Coulomb interaction is relatively small. For this, to hold the electron gas must be appropriately dense, so, as to satisfy the condition $k_F \gg a_0^{-1}$, where k_F is the one-dimensional Fermi momentum and a_0 - the effective Bohr radius**.** In the case of the "size quantum limit" when only one subband is filled, $k_F = \pi N_l/2$ and the foregoing condition of the weak nonideality of the plasma can be written in the form $N_l a_0 \gg 1$ i.e. the number of electrons on the spatial interval of a Bohr orbit should be large. Our theory applies only to this case.

Subsequently, here we deal a with dielectrically heterogeneous QWr structure. It is necessary to take into account the electrostatic image forces. The energy of the Coulomb interaction between the charges $-e$ and e (e - is the electron charge) to be located at (0,0) and (ρ, z) points in a QWr can be found by solving the Poisson equation with appropriate boundary conditions. The general solution with axial symmetry and reflection symmetry in the origin inside the QWr is [7]

$$V(\rho, z) = \frac{2}{\pi}\int_0^\infty cosqzV(\rho, q)dq \,, \tag{1}$$

where the Fourier component in (1) is equal to

$$V(q,\, \rho) = -\frac{e^2}{\varepsilon_s}\left[K_0(q\rho) + \frac{(\varepsilon_r - 1)K_0(qR)K_1(qR)I_0(q\rho)}{\varepsilon_r K_0(qR)I_1(qR) + K_1(qR)I_0(qR)}\right], \tag{2}$$

and $\varepsilon_r = \varepsilon_w / \varepsilon_b$, K_i and I_i $(i = 0, 1)$ are the modified Bessel functions.

In order to get a general qualitative insight into the "Coulomb interaction engineering" possibilities of the strong DC effect, a strong contrast between dielectric constants is accepted ($\varepsilon_r = \varepsilon_w / \varepsilon_b \gg 1$) and the strong confinement condition $a_0 \gg R$ is assumed. Under these circumstances in Exps.(1) and (2), an important role will be played by 1D distances of $z >> R$ for that there exists in the 1D wave vector, a q interval so that $q\ R << 1$ and the expansion of Exp.(2) up to the lowest order in this small parameter gives:

$$V(q) = -\frac{e^2}{\varepsilon_s}\left[ln(qR)^{-1} + \frac{(\varepsilon_r-1)ln(qR)^{-1}}{\varepsilon_r(qR)^2 ln(qR)^{-1}+1}\right]. \tag{3}$$

The 1D EG longitudinal dispersion spectrum of unretarded intraband plasmons with the DC effect in QWr was previously discussed in [4] by using the random phase approximation (RPA) and in accordance with that, the collective modes are obtained from the secular equation:

$$1 - \Pi_0 V(q) = 0\ , \tag{4}$$

where

$$\Pi_0 = \frac{N_l q^2}{m_e \omega^2}\ , \tag{5}$$

is the usual polarization propagator for a 1D EG, $m_e = m_{l(t)}$, ω is the 1D EG plasmon mode frequency. The root for Exp.(4) would be calculated by combining Exps.(3), (5) and (4). As a result the expression

$$\omega_{pl}^{1D} = \left(\frac{2N_l e^2}{\varepsilon_s m_e R^2}\right)^{\frac{1}{2}} (qR)\left[ln(qR)^{-1} + \frac{(\varepsilon_r-1)ln(qR)^{-1}}{\varepsilon_r(qR)^2 ln(qR)^{-1}+1}\right]^{\frac{1}{2}} \tag{6}$$

is the unretarded intrasubband plasmon frequency, which involves 1D EG oscillations parallel to the QWr axis including the DC effect. In view of the restrictions $qR << 1$ and $\varepsilon_r \gg 1$, there are two distinct ranges for the 1D wave vector q such as

$$a)\ \varepsilon_r(qR)^2 ln(qR)^{-1} \ll 1 \text{ and } b)\ \varepsilon_r(qR)^2 ln(qR)^{-1} \gg 1\ , \tag{7}$$

that Exp.(6) goes to the final form as

$$a)\ \omega_{pl}^{1D} = \left(\frac{2N_l e^2}{\varepsilon_b m_e}\right)^{\frac{1}{2}} q\ [ln(qR)^{-1}]^{\frac{1}{2}}\ , \tag{8a}$$

$$b)\ \omega_{pl}^{1D} = \left(\frac{2N_l e^2}{\varepsilon_s m_e R^2}\right)^{\frac{1}{2}}. \tag{8b}$$

Exps.(7,8) obtained already in [5] describes the Q1D plasmon mod dispersion spectrum in QWr in presence of strong DC effect. They really differs from the results of [3] since in the latter a strong DC effect specific influence on the collective plasmon modes in QWr has been ignored and thus quite characteristic analytical features of Exp.(8b) such as

1) the plasmon frequency for "moderately" small wave vectors explicitly is independent of q,

2) the plasmon frequency for "moderately" small wave vectors strongly depending on R, are omitted.

3. Numerical results and conclusion. The Q1D EG plasmon mode theory presented here applies heterogeneous QWr systems with large differences of dielectric constants for the neighbouring media. At present, corresponding experimental works on such realistic systems exist. In particular, reported in [8] , a free-standing PbSe-based QWr system is a good prospect related to a strong DC effect due to large values of dielectric constant ($\varepsilon_w \approx 250$). Based on this, the feasibility of the presented theoretical model will be described for this particular structure.

So, let us now carry out the Q1D collective plasmon mode numerical calculations of the realistic PbSe/vacuum QWr system. For the dielectric constants' ratio $\varepsilon_r = \varepsilon_w/\varepsilon_b = \varepsilon_{PbSe}/\varepsilon_{vacuum} \approx 250 / 1 = 250$ value is taken [4]. Note that the PbSe bulk sample holds the smallest electron effective mass ($m_l \approx 0.071 m_0$, $m_t \approx 0.041 m_0$ m_0 - is the free electron mass)) and the macroscopically large effective Bohr radius ($a_{0l} \approx 188$ nm, $a_{0t} \approx 325$ nm). With this, in accordance whit the strong QC condition $a_0 >> R$, we will display the numerical data for the QWr radius values $R<15$ nm and for typical moderate high ($\sim 10^6$ cm^{-1}) 1D densities. Figure 1 shows the unretarded collective excitation dispersion curves of the intrasubband Q1D plasmons where the plasmon frequency ω_{pl}^{1D} (scaled in terms of 10^{13}s units) is plotted as a function of the qR in accordance with Exp.(6). Correspondingly, the following dispersion graphs are displayed here:

a1)The Q1D plasmon mode in the dielectrically homogeneous ($\varepsilon_w \approx \varepsilon_b$) PbSe-based QWr system with $m_e = m_t$ - dotted line,

a2)The Q1D plasmon mode in the strong DC-affected ($\varepsilon_w \approx 250, \varepsilon_b = 1$) PbSe-based

QWr system with $m_e = m_l$ - dashed-dotted line,

a3) The Q1D plasmon mode in the strong DC-affected ($\varepsilon_w \approx 250, \varepsilon_b = 1$) PbSe- based QWr system with $m_e = m_t$ - thin solid line,

b) The Q1D plasmon mod in the dielectrically homogeneous ($\varepsilon_w \approx \varepsilon_b \approx 12.5$) GaAs- based QWr system with $m_e \approx 0.071 m_0$ - bold solid line,

c) The Q1D plasmon mode in weak DC-affected ($\varepsilon_w \approx 17.7, \varepsilon_b = 2.5$) InSb -based QWr system with $m_e \approx 0.014 m_0$ - bold dashed line.

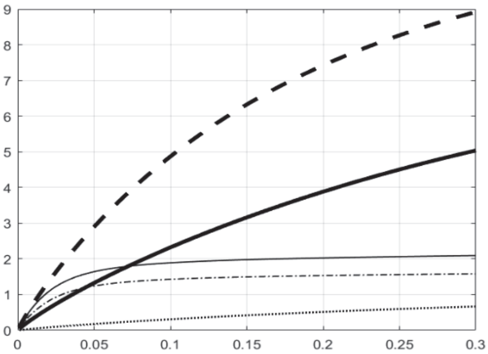


Fig. 1. The Q1D plasmon collective modes frequency with $R \approx 5$ *nm,* $n_l \approx 2.10^6$ *cm*$^{-1}$ *as a function of the wave vector for the PbSe/vacuum QWr system (*ω_{pl}^{1D} *is in units of* 10^{13}*s)*

Following to the dispersion graphs after ***a1), a2)*** and ***a3)*** in Fig.1, the DC effect essentially enhances the Q1D plasmon mode frequency (on the average by 5-8 times). At the same time, as follows from the dispersion graphs after ***a1), b)*** and ***c)*** in Fig.1, both for the DC effect absent and weakly expressed cases the Q1D plasmon modes are described wholly by Exp.(8a). In turn, in accordance with the dispersion graphs after ***a2)*** and ***a3)*** in Fig.1, when the DC effect is expressed strongly, the Q1D plasmon modes are characterized by Exp.(8a) which takes place for quite narrow ranges of the wave vectors (qR<0.05). While for the dominant part of the long wave-related q vector values (0.05< qR<0.3) the Q1D plasmon modes are characterized by Exp.(8b). Graphically, this looks as the dispersion curve specific "saturation" and the latter here starts quite fast for the graph after ***a3)*** than ***a2)*** which is due to the differences between the transverse and longitidunal effective masses for electrons of the PbSe material.

Thus, we may ascertain that just for the definite QWr system with a strongly expressed DC effect (in discussing the case with a PbSe-based realistic QWr system) the Q1D plasmon modes could be independent explicitly of the wave vector.

REFERENCES

1. **Das Sarma S., Lai Wu-yan.** Screening and elementary excitations in narrow-channel semiconductor microstructures // Physical.Review.B .- 1985.-V.32.-P. 1401.
2. **Aharonyan K.H., Margaryan N.B.** Dielectric confinement influenced screened Coulomb potential for a semiconductor quantum wire // Journal of Physics: Conference Series.-2016.-V.672.-P. 012009-8.
3. **Wendler L., Grigoryan V.G.** Optical and acoustic plasmons in cylindrical quantum-well wires // Physical.Review.B .- 1994.-V.49.-P. 14531.
4. **Aharonyan K.H., Erknapetyan H.L., Tilley D.R.** Collective plasmon modes in thin semiconductor films including the effect of the image charges // Physica status solidi (b).- 1988.-V.150.-P. 133.

5. **Aharonyan K.H., Khachatryan A.Zh.** Collective plasmon modes in quantum wires including the effect of the image charges // National Polytechnic University of Armenia Bulletin, Collection of Scientific Papers.- 2004.-V.1.-P. 45.
6. **Aharonyan K.H., Sedrakyan D.G.** Collective plasmon modes in semiconductor superlattice structures in presence of the image charges // Physica status solidi (b).-1991.-V.164.-P. 127.
7. **Ivanenko D.D., Sokolov A.A**. Classical field theory // GTTI.-1951.
8. **Lifshitz E., Bashouti M., Kloper V., Kigel A., Eisen M. S., Berger S.** Synthesis and Characterization of PbSe Quantum Wires, Multipods, Quantum Rods, and Cubes // Nanoletters.-2003.- V.3.-P. 857.

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ՊԼԱԶՄՈՆԱՅԻՆ ՏԱՏԱՆՈՒՄՆԵՐԻ ԱՌԱՆՁՆԱՀԱՏԿՈՒԹՅՈՒՆՆԵՐԸ PbSe ՀԵՆՔՈՎ ԱԶԱՏ ՏԵՂԱԿԱՅՎԱԾ ԿԻՍԱՀԱՂՈՐԴԱՅԻՆ ՔՎԱՆՏԱՅԻՆ ԼԱՐԵՐՈՒՄ

Ազատ տեղակայված իրական PbSe քվանտային լարում քննարկված են քվազիմիաչափ պլազմոնային տատանումների դիսպերսիոն սպեկտրի առանձնահատկությունները դիէլեկտրական ուժեղ կապակցման երևույթի առկայությամբ: Ցույց է տրված, որ այդպիսի նանոհամակարգում, բացի երկարալիքային սահմանին վերաբերող պլազմոնային ներենթագոտիական տատանումներից, կարող են նաև իրականանալ այլընտրանքային երկարալիքային տատանումներ, որոնց հաճախությունը կախված չէ ալիքային վեկտորից և միաժամանակ աճում է լարի հաստության նվազմանը զուգահեռ: Կատարված է պլազմոնային թույլատրելի սպեկտրային բնութագրական տիրույթի թվային վերլուծություն:

Առանցքային բառեր. ազատ տեղակայված PbSe քվանտային լար, պլազմոն, դիսպերսային սպեկտր:

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ОСОБЕННОСТИ ПЛАЗМЕННЫХ КОЛЛЕКТИВНЫХ МОД В СВОБОДНО СТОЯЩИХ ПОЛУПРОВОДНИКОВЫХ КВАНТОВЫХ НИТЯХ НА БАЗЕ PbSe

Обсуждаются особенности дисперсионного спектра квазиодномерных плазменных мод в свободно стоящих квантовых нитях на базе PbSe при наличии сильного диэлектрического разрыва. Показано, что в такой наносистеме, помимо плазменных внутризонных колебаний на длинноволновом пределе, могут возникать альтернативные длинноволновые колебания, частота которых не зависит от волнового вектора и одновременно увеличивается с уменьшением толщины нити. Проведен численный анализ разрешенной спектральной характеристической области плазмонов.

Ключевые слова: свободно стоящая квантовая нить, плазмон, дисперсионный спектр.