CALCULATION OF EXCITONIC ABSORPTION SPECTRUM OF GaAs QUANTUM WIRE FREE-STANDING IN VACUUM

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The electron–hole interaction in a thin (≈ 10 nm) GaAs quantum wire free-standing in vacuum is strongly enhanced by the image charge due to the abrupt permittivity drop at the wire surface. As a result, the exciton binding energies are much larger and the exciton wave functions much more localised than those of the GaAs quantum wire surrounded by the AlGaAs. The absorption spectrum of the free-standing wire shows besides the $1s$ exciton peak also the $3s$ and $5s$ exciton peaks, even if the peaks are 15 meV broad. The continuum absorption edge shows a large blue shift due to the renormalization of single-particle energies by the image charge.

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The free-standing quantum wells and wires are thin films, bars, or whiskers supported only on their ends or connected to the substrate only on the side with the smallest cross-section [1]. In thin (≈ 10 nm) structures the electron–hole (e–h) Coulomb interaction is enhanced by the image charge due to the small permittivity of the surrounding medium (vacuum or air). We have shown [2] that in a thin free-standing GaAs quantum well the enhanced e–h interaction enhances the exciton binding energy by almost one order of magnitude compared to the AlGaAs/GaAs/AlGaAs quantum well. As a result the absorption spectrum is strongly modified: the $2s$ and $3s$ exciton peaks are distinguished in addition to the $1s$ peak, and the continuum absorption edge shows a large blue shift due to the renormalization of single-particle energies by the image charge. In free-standing wires these effects can be expected to be stronger, as supported by recent calculations of exciton binding energies [3]. In this work we verify these expectations by calculating the absorption spectrum of a cylindrical GaAs quantum wire free-standing in vacuum.

We start with the derivation of the e–h interaction energy. We consider an undoped infinitely long wire with a cylindrical cross-section in the y–z plane and with the wire axis associated with the x-axis. At the wire surface there is an abrupt

permittivity drop from $\epsilon_s = 12.5\epsilon_0$ to ϵ_0, where ϵ_s and ϵ_0 are the permittivities of GaAs and vacuum, respectively. Assuming at the wire surface an infinitely high potential barrier, the envelope function of the carrier ground state is given in the effective mass approximation as $\psi_{11}(r) = J_0\left(x_{01}\frac{r}{R}\right) / [\sqrt{\pi}RJ_1(x_{01})]$, where J_0, J_1 are the Bessel functions, x_{01} is the first zero of the J_0, $r = \sqrt{y^2 + z^2}$, and R is the wire radius. The corresponding carrier charge density is $\rho(r) = e|\psi_{11}(r)|^2$. The potential $\varphi(x - x_h, r)$ created at point x, r inside the wire by that charge density (say by a hole positioned at $x = x_h$) obeys the Poisson equation

$$\nabla[\epsilon(r)\nabla\varphi(x - x_h, r)] = -\rho(r)\delta(x - x_h),$$

where $\epsilon(r) = \epsilon_0 + (\epsilon_s - \epsilon_0)\theta(R - r)$ and $\theta(R - r)$ is the Heaviside step function. The Poisson equation in cylindrical coordinates reads

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}\right)\varphi(x - x_h, r) = -\frac{\rho(r)}{\epsilon_s}\delta(x - x_h) - \frac{\rho_{im}(x - x_h, r)}{\epsilon_s}, \quad (1)$$

$$\rho_{im}(x - x_h, r) = \left(\frac{\epsilon_s}{\epsilon(r)} - 1\right)\rho(r)\delta(x - x_h) + \frac{\epsilon_s}{\epsilon(r)}\frac{\partial\epsilon(r)}{\partial r}\frac{\partial\varphi(x - x_h, r)}{\partial r}, \quad (2)$$

where $\rho_{im}(x - x_h, r)$ is the image charge density. The Fourier transform of (1) gives

$$\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} - Q_x^2\right)\varphi(Q_x, r) = -\frac{\rho(r)}{\epsilon_s} - \frac{\rho_{im}(Q_x, r)}{\epsilon_s}, \quad (3)$$

where

$$\varphi(Q_x, r) = \int_{-\infty}^{\infty} d(x - x_h)e^{iQ_x(x - x_h)}\varphi(x - x_h, r)$$

and

$$\rho_{im}(Q_x, r) = \int_{-\infty}^{\infty} d(x - x_h)e^{iQ_x(x - x_h)\rho_{im}}(x - x_h, r).$$

The solution of (3) with the right hand side replaced by $\delta(r - r_0)$ is the Green function $G(Q_x, r, r_0) = -I_0(Q_xr^<)K_0(Q_xr^>)$, where I_0 and K_0 are the modified Bessel functions, $r^< = \min(r, r_0)$, and $r^> = \max(r, r_0)$. The general solution of (3),

$$\varphi(Q_x, r) = \int_0^\infty dr_0 r_0 G(Q_x, r, r_0)[-\rho(r_0) - \rho_{im}(Q_x, r_0)]/\epsilon_s,$$

allows us [4] to derive

$$\varphi(Q_x, r) = -\frac{e}{\epsilon_s}\left[G_{11}(Q_x, r) + \frac{\epsilon_s - \epsilon_0}{\epsilon_0}\frac{RG(Q_x, r, R)\frac{\partial G_{11}(Q_x, r=R)}{\partial r}}{1 - \frac{\epsilon_s - \epsilon_0}{\epsilon_0}R\frac{\partial G(Q_x, r=R, R)}{\partial r}}\right], \quad (4)$$

where $G_{11}(Q_x, r) = \int_0^R dr_0 r_0 G(Q_x, r, r_0)|\psi_{11}(r_0)|^2$. Finally, the effective e–h interaction

$$-e\varphi_{e-h}^{eff}(x_e - x_h) = -e\int_{-\infty}^{\infty} dQ_x e^{-iQ_x(x_e - x_h)}\varphi_{11}(Q_x), \quad (5)$$

is the inverse Fourier transform of the function $\varphi_{11}(Q_x) = \int_0^R dr\, r\varphi(Q_x, r)$ $\times |\psi_{11}(r)|^2$. The second term on the right hand side of (4) is the potential due to

the image charge ρ_{im}. It disappears when $\epsilon_0 \rightarrow \epsilon_s$, i.e., when the wire is buried in the AlGaAs (we ignore a small difference between the permittivity of GaAs and AlGaAs).

When the wave function of the e–h pair, $\Psi(x_e - x_h, r_e, r_h)$, is approximated as $\psi_{11}(r_e) \psi_{11}(r_h) \Phi(x_e - x_h)$, the eigenenergy of the e–h pair can be expressed as

$$E_g = E_0 + \frac{\hbar^2}{2}\left(\frac{1}{m_e} + \frac{1}{m_h}\right)\left(\frac{x_{01}}{R}\right)^2 + \sigma_e + \sigma_h - E_b, \tag{6}$$

where E_b and $\Phi(x)$ satisfy the equation

$$\left[-\frac{\hbar^2}{2}\left(\frac{1}{m_e} + \frac{1}{m_h}\right)\frac{\partial^2}{\partial x^2} - e\varphi_{e-h}^{eff}(x)\right]\Phi(x) = -E_b\Phi(x). \tag{7}$$

Here E_0 is the energy gap of bulk GaAs, $\frac{\hbar^2}{2}\left(\frac{1}{m_e} + \frac{1}{m_h}\right)(x_{01}/R)^2$ is the carrier confinement energy, σ_e and σ_h are the electron and hole selfenergies (Eq. (9)), and E_b is the exciton binding energy. The electron and hole effective masses, m_e and m_h, are taken as $0.067m_0$ and $0.2m_0$. In the two-band model the choice $m_h = 0.2m_0$ fits the dispersion of the ground hole subband resulting from the heavy and light hole mixing [5].
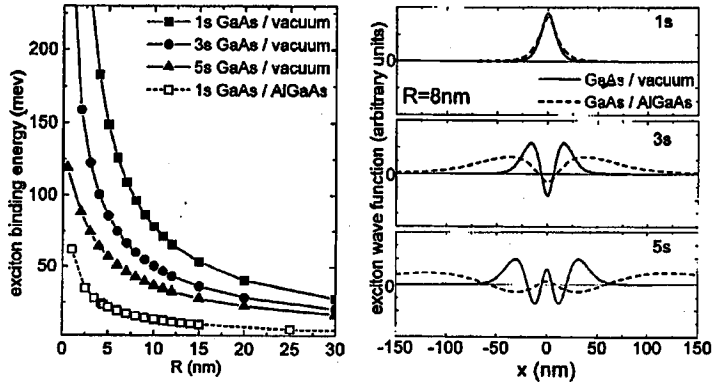

Fig. 1.   The exciton binding energy versus the wire radius R and the exciton wave function for $R = 8$ nm. Three lowest states with even wave functions (labelled $1s$, $3s$, $5s$) are shown. The solid lines are the results for the free-standing GaAs wire, the dashed lines are the results for the GaAs wire buried in the AlGaAs.

Figure 1 shows the exciton binding energy versus the wire radius R and the exciton wave function $\Phi(x)$ for $R = 8$ nm. The solid lines are the results for the free-standing GaAs wire, the dashed lines are the results for the GaAs wire buried in the AlGaAs. Only the three lowest states with even wave functions (labelled $1s$, $3s$, $5s$) are shown, since mainly these states contribute to the excitonic absorption. In the free-standing wire the binding energies are much larger and the wave functions are more localized. This is due to the enhanced e–h interaction (see Fig. 2). Figure 2 shows the effective e–h interaction energy $-e\phi_{e-h}^{eff}$ versus the e–h

distance x for the wire radius $R = 8$ nm. The thick solid line is obtained for the free-standing wire, the thick dashed line for the buried wire. In the former case the e–h interaction is much stronger, which is due to the image charge effect (the second term on the right hand side of (4)). In the latter case the effect disappears.
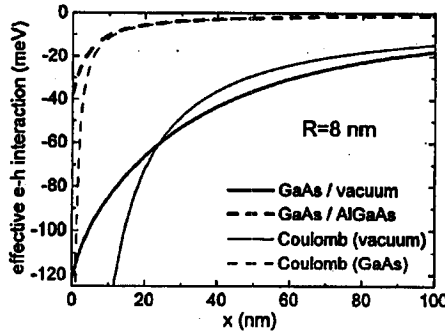

Fig. 2. The effective e–h interaction energy versus the e–h distance for the wire radius $R = 8$ nm. The thick solid line is the result for the free-standing GaAs wire, the thick dashed line for the buried GaAs wire. Also shown is the Coulomb e–h energy of two point-like charges in vacuum (thin solid line) and in GaAs (thin dashed line).

The absorption coefficient of the quantum wire versus the photon energy (E) reads [6]

$$\alpha = \frac{\xi_1}{E} \frac{\theta\left(E - E'_g\right)}{\sqrt{E - E'_g}} + \frac{\xi_2}{E} \sum_{i=1}^{\infty} \delta\left(E - E'_g + E_{b,i}\right) |\Phi_i\left(x = 0\right)|^2, \qquad (8)$$

where E'_g is the energy of the continuum edge (the right hand side of (6) without E_b), the sum extends over all the bound exciton states,

$$\xi_1 = \left(P^2 e^2 \sqrt{2\mu}\right) / \left(2\epsilon_0 c n_r m_0^2 \pi R^2\right),$$

$$\xi_2 = \left(P^2 e^2 \pi \hbar\right) / \left(\epsilon_0 c n_r m_0^2 \pi R^2\right),$$

P is the matrix element between the valence band p state and the conduction band s state at Γ for GaAs $(P^2/m_0 = 11.3\,\text{eV})$, $n_r = 3.7$ is the refraction index of GaAs, and $\mu = m_e m_h / (m_e + m_h)$. The first and second terms in (8) describe the continuum and the exciton contribution, respectively. Since the first term is derived [6] in the single electron approximation, it should be multiplied by the Sommerfeld factor. Here we use the Sommerfeld factor values taken from Fig. 2b of Ref. [7]. Since these values were obtained for a buried GaAs wire, they likely overestimate the Sommerfeld factor of the free-standing wire. We also incorporate the inhomogeneous broadening by convoluting the spectrum (8) with a Gaussian function $\exp\left[-\left(E'_g - \langle E'_g \rangle\right)^2 / \left(2\Delta E'^{\,2}_g\right)\right]$, where $\langle E'_g \rangle$ and $\Delta E'_g$ are the mean value and the mean deviation of E'_g.

In Fig. 3 we compare the absorption spectra of the free-standing wire and buried wire. The broadening $2\Delta E'_g = 10$ meV is considered here. The distance between the $1s$ exciton peak and the onset of the continuum is the $1s$ exciton
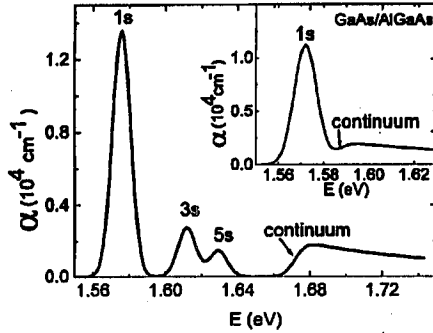
Fig. 3.   Absorption coefficient of the free-standing GaAs quantum wire with 8 nm radius. The inset shows the spectrum of the buried GaAs quantum wire.

binding energy. It is 6.5 times larger for the free-standing wire than for the buried wire. For the former case also the $3s$ and $5s$ peaks are visible. The $5s$ peak tends to smear out when $2\Delta E_g' > 15$ meV. Another remarkable feature is the 84 meV blue shift of the free-standing wire spectrum. The blue shift is determined by the $\sigma_e + \sigma_h$. The selfenergy σ_γ, $\gamma = e, h$, is the increment of the carrier energy due to the image charge. It is given as

$$\sigma_\gamma = 2\pi \int_0^R \mathrm{d}r_\gamma r_\gamma \sigma_\gamma (r_\gamma) |\psi_{11}(r_\gamma)|^2, \tag{9}$$

where $\sigma_\gamma (r_\gamma) = (e/2) \int_{-\infty}^{\infty} \mathrm{d}Q_x \int_0^R \mathrm{d}r \, r|\psi_{11}(r)|^2$ (second term on the right hand side of (4)).

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