Excitons in a GaAs Film on $Al_xGa_{1-x}As$ Influenced by the Thickness of the Substrate

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Within the framework of the fractional-dimensional approach, exciton binding energies in GaAs films on $Al_xGa_{1-x}As$ substrates are investigated theoretically. In this scheme, the real anisotropic "exciton + film" semiconductor system is mapped into an effective fractional-dimensional isotropic space. For different aluminum contents and film thicknesses, the exciton binding energies are obtained as functions of the substrate thickness. The numerical results shown that, for different aluminum contents and film thicknesses, the exciton binding energies in GaAs films on $Al_xGa_{1-x}As$ substrates all exhibit their maxima as the substrate thickness increases. It is also shown that the binding energies of heavy-hole and light-hole excitons both have their maxima as the substrate thickness increases.

1. Introduction

In recent years there has been considerable interest in the physics nature of exciton, polaron and impurity properties of semiconductor heterostructures, such as quantum wells, quantum wires, quantum dots, superlattices, films on substrates, etc. Such interest has arisen due to the physics nature underlying various properties of these systems and potential applications in the wide range of electronic and optoelectronic devices. In fact, excitons have great effects on a variety of physical phenomena observed in these structures. Therefore an understanding of these properties such as the increase in exciton binding energy due to confinement of the carriers has become an important topic in the physics of low-dimensional structures during the past decades. Plenty of work was devoted to study the excitonic properties in films theoretically and experimentally. Several authors have calculated binding energies of excitons in free-standing GaAs films by using variational schemes [1]. Optical spectroscopy of large-momentum excitons in GaAs films was experimentally and theoretically investigated by some authors [2, 3]. Photoluminescence (PL) spectrum measurements was used to treat exciton [4, 5] and exciton-polaritons [6] problems and to determine the exciton binding energy [7, 8] in various semiconductor films such as CdS, ZnSe, GaN and $CsSnI_3$ films. In particular, the GaAs film on $Al_xGa_{1-x}As$ substrate is an important semiconductor low-dimensional structure.

We perform our study based on the fractional-dimensional approach (FDA) first proposed by He [9, 10] to study excitons and optical properties of anisotropic

solids. In this scheme, the Schrödinger equation is solved in a noninteger-dimensional space where the interactions are assumed to occur in an isotropic effective environment, and the fundamental quantity is the fractional dimension D associated with the effective medium, and with the degree of anisotropy of the actual system. In the last few years, the FDA has been successfully used in the study of the excitons [11–15], biexcitons [16–18], magnetoexciton [19–21], excitonic and impurity states [20, 22–27], polarons [28–31], exciton–phonon interaction [32–35] in anisotropic semiconductor heterostructures. However, as far as we know, the FDA has not been extended to study excitons in a GaAs film on $Al_xGa_{1-x}As$ substrate.

We have studied the polaron effect in a GaAs film deposited on $Al_xGa_{1-x}As$ substrate within the FDA [36, 37]. In this paper, we extend the FDA to the case of an exciton confined to a GaAs film on $Al_xGa_{1-x}As$ substrate. Within the FDA, the system "exciton + GaAs film" is practically described by an equivalent isotropic hydrogenic system in a fractional D-dimensional space, a problem which can be solved analytically. As functions of the substrate thickness, the exciton binding energies are calculated. This paper is organized as follows. In Sect. 2 the theoretical framework of the FDA is extended to the case of excitons confined in GaAs films on $Al_xGa_{1-x}As$ substrates. Numerical results and discussion are in Sect. 3, and conclusions are in Sect. 4.

2. Theoretical framework

We consider the problem of an exciton confined in a GaAs film on $Al_xGa_{1-x}As$ substrate (growth axis along the z direction). For the case of no electron and hole escaping from the system, the potentials of the GaAs film–$Al_xGa_{1-x}As$ substrate are characterized by

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$$V_j(z_j) = \begin{cases} V_f(= 0) & \text{if} \quad 0 \leq z_j \leq L_f, \\ V_{sj} & \text{if} \quad L_f < z_j < L_f + L_s, \\ \infty & \text{otherwise,} \end{cases} \quad (1)$$

where $j =$ e, h represent the electron and hole, respectively. L_f and L_s represent the film thickness and substrate thickness, respectively, and the subscripts f and s label the film (GaAs) and substrate ($Al_xGa_{1-x}As$) regions, respectively.

Within the FDA proposed by He [9, 10], the exciton problem in an anisotropic solid can be treated as one in an isotropic fractional-dimensional space whose dimension D depends on the degree of anisotropy of the actual system, the discrete bound-state energies and orbital radii are given by

$$E_n = E_g - \frac{E_0}{\left[n + \frac{D-3}{2}\right]^2},$$
$$a_n = a_0 \left[n + \frac{D-3}{2}\right]^2, \quad (2)$$

where D is the dimension of a solid, $n = 1, 2, ...$ is the principal quantum number, E_0 and a_0 are the effective Rydberg constant and effective Bohr radius, respectively, $E_0 = (\varepsilon_0/\varepsilon)^2(\mu/m_0)R_H$ and $a_0 = (\varepsilon/\varepsilon_0)(m_0/\mu)a_H$, where R_H and a_H are the Rydberg constant and Bohr radius, respectively, m_0 is the free-electron mass and μ is the exciton reduced mass $1/\mu = 1/m_e + 1/m_h$.

According to Eq. (2) and in the case of our GaAs film–$Al_xGa_{1-x}As$ substrate system, the binding energy of the $1s$ exciton can be written as

$$E_b = \left(\frac{2}{D-1}\right)^2 E_0^*, \quad (3)$$

where E_0^* is the mean value of the effective Rydberg energy for the three-dimensional (3D) exciton which can be written as

$$E_0^* = \left(\frac{\varepsilon_0}{\varepsilon^*}\right)^2 \left(\frac{\mu^*}{m_0}\right) R_H, \quad (4)$$

where ε^* is the mean value of dielectric constant of GaAs film–$Al_xGa_{1-x}As$ substrate material, μ^* is the mean value of exciton reduced mass. In Eq. (3), D = 3, 2, or 1 give, respectively, $E_b = E_0^*, 4E_0^*$, or ∞, corresponding to the well-known results of the integer-dimension models.

In our GaAs film–$Al_xGa_{1-x}As$ substrate system, within the effective mass and parabolic band approximations the Hamiltonian for the single electron ($j =$ e) or hole ($j =$ h) may be given by

$$H_j = -\frac{\hbar^2}{2} \frac{d}{dz_j} \left(\frac{1}{m_j(z_j)} \frac{d}{dz_j}\right) + V_j(z_j), \quad (5)$$

where $m_j(z_j)$ represent the z-dependent (film or substrate) effective masses of the electron ($j = e$) and hole ($j = h$), respectively,

$$m_j(z_j) = \begin{cases} m_{fj} & \text{if} \quad 0 \leq z_j \leq L_f, \\ m_{sj} & \text{if} \quad L_s < z_j < L_f + L_s, \\ 0 & \text{otherwise.} \end{cases} \quad (6)$$

The dimensional parameter D that guarantees the mapping of the real system into the fractional-dimensional space can be calculated through the relation [28]:

$$D = 3 - \exp(-\xi), \quad (7)$$

where ξ represents the ratio of the length of confinement to the effective characteristic length of interaction.

In the case of an exciton confined in a GaAs film on $Al_xGa_{1-x}As$ substrate, the exciton is no longer restricted to the region inside the film only. Therefore, the spreading of the exciton wave function into the substrate has to be considered in defining the corresponding length of confinement. Taking into account the spatial extension of the exciton motion in the substrate region, the length of confinement is characterized by an effective film thickness L_f^* which may be written as

$$L_f^* = L_f + \frac{1}{k_{se}} + \frac{1}{k_{sh}}, \quad (8)$$

where k_{se} and k_{sh} represent the electron and hole wave vectors in the substrate region, respectively. k_{se} and k_{sh} are given by

$$k_{sj} = \frac{\sqrt{2m_{sj}(V_{sj} - E_j)}}{\hbar}, \quad (9)$$

where E_j being the electron ($j =$ e) or hole ($j =$ h) eigenenergies determined by H_j [see Eq. (5)].

On the other hand, the effective length that characterizes the electron–hole interaction is the mean value of the effective Bohr diameter of the 3D exciton

$$d_0^* = 2a_0^* = 2\frac{\varepsilon^*}{\varepsilon_0} \frac{m_0}{\mu^*} a_H, \quad (10)$$

where a_0^* is the mean value of the effective Bohr radius.

Therefore, the dimensional parameter D can be calculated through the relation

$$D = 3 - \exp\left(-\frac{L_f^*}{2a_0^*}\right). \quad (11)$$

In a GaAs film–$Al_xGa_{1-x}As$ substrate system, the material parameters which characterize the exciton properties differ when passing from the film to the substrate region. In other words, the effective-mass mismatch between the film and substrate materials should be considered. In order to take account of this fact, we may assign the effective fractional-dimensional space an average of the material parameters over the exciton positions. The mean values of the material parameters can be calculated in the same manner as in Ref. [38]. Our effective fractional-dimensional electron–hole interaction is then characterized by the following mean values of the material parameters:

$$\left(m_j^*\right)^{-1} = \sum_{i=f,s} \frac{P_{ij}}{m_{ij}}, \quad (12)$$

and

$$\varepsilon^* = \sum_{i=f,s} P_i \varepsilon_i. \quad (13)$$

In Eq. (13) ε_i represent the material dielectric functions in the different regions, and

$$P_{fj} = \int_0^{L_f} |\Psi_j(z_j)|^2 \, dz_j,$$

$$P_{sj} = 1 - P_{fj} \tag{14}$$

denote the probabilities of finding the single electron (j = e) or hole (j = h) in the film and substrate regions, respectively. Finally, the binding energy of an exciton confined in a GaAs film on $Al_xGa_{1-x}As$ substrate can be obtained in an analytical way from Eqs. (3), (4) and (11) and assuming the mean values of the material parameters defined in Eqs. (12)–(14). We use in our calculations the same set of material parameters as discussed by Smondyrev et al. [38]. The numerical results and discussion are in Sect. 3.

3. Numerical results and discussion

The binding energy of the heavy-hole exciton in the GaAs film on $Al_xGa_{1-x}As$ substrate, as a function of the substrate thickness, is shown in Fig. 1, for different Al contents at the film thickness $L_f = 10$ Å. As can be seen, exciton binding energy starts from the same value $E_b = 15.4$ meV corresponding to the value of a infinite quantum well with a well width $L_w = 10$ Å. The binding energies first increase as the substrate thickness increases for different Al contents and reach maxima at the substrate thicknesses $L_s \approx 13$ Å for $x = 0.1$, $L_s \approx 21$ Å for $x = 0.3$, and $L_s \approx 23$ Å for $x = 0.5$, respectively. By continuing to increase the substrate thickness, the binding energies then decrease gradually. We note that increasing the Al content will make the maximum value of the binding energy move to the thicker substrate thickness.
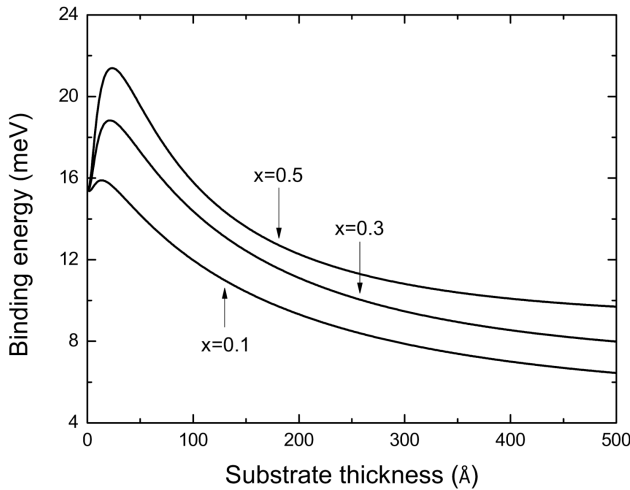

Fig. 1. The heavy-hole exciton binding energy in the GaAs film on $Al_xGa_{1-x}As$ substrate as a function of the substrate thickness for different Al contents at the film thickness $L_f = 10$ Å.

The fractional dimension D corresponding to the fractional-dimensional result in Fig. 1 is displayed in Fig. 2, as a function of the substrate thickness. It can be seen that, the fractional dimension starts from the same value D ≈ 2.06 corresponding to the value of a infinite quantum well with a well width $L_w = 10$ Å. Note that the fractional dimension increases monotonously as the substrate thickness increases. As the substrate thickness increases, the confinement becomes more and more weak, leading to an increase in the fractional dimension that has the limit value D= 3.
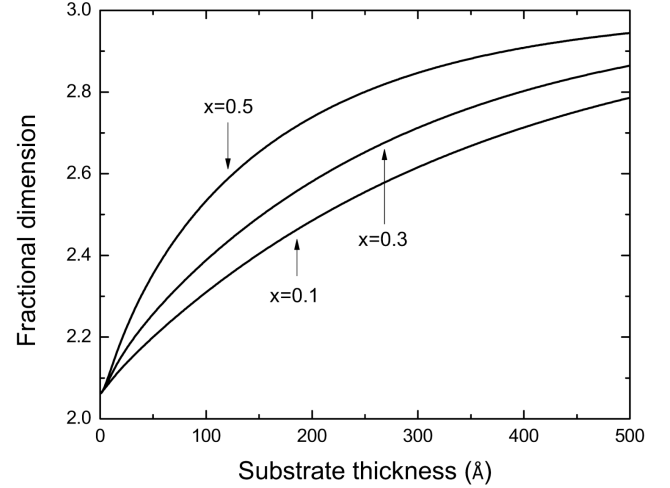

Fig. 2. The corresponding fractional dimension D as a function of the substrate thickness for different Al contents at the film thickness $L_f = 10$ Å.

The binding energy of the heavy-hole exciton in the GaAs film on $Al_{0.3}Ga_{0.7}As$ substrate, as a function of the substrate thickness, is shown in Fig. 3, at different values of the film thickness $L_f = 7, 10, 13$ Å, respectively. It can be seen that, for different values of the film thickness, the exciton binding energy have a maximum as the substrate thickness increases. The maxima appear at the substrate thickness $L_s \approx 17, 21, 23$ Å, respectively. We note that the exciton binding energy decreases with increase of the film thickness. It is also worth remarking that different film thicknesses have significant influence on the exciton binding energy for thin and medium substrate thicknesses but have no significant influence for extremely thick substrate thicknesses.

The fractional dimension D corresponding to the fractional-dimensional result in Fig. 3 is displayed in Fig. 4, as a function of the substrate thickness. For the case of different values of the film thickness, the fractional dimensions all increase monotonously as the substrate thickness increases. The values of the fractional dimension start from D ≈ 2.04 for $L_s = 7$ Å, D ≈ 2.06 for $L_s = 10$ Å and D ≈ 2.08 for $L_s = 13$ Å, respectively. As the substrate thickness increases, the confinement becomes more and more weak, leading to an increase in the fractional dimension that has the same limit value D= 3. We note that the fractional dimension decreases with decrease of the film thickness.
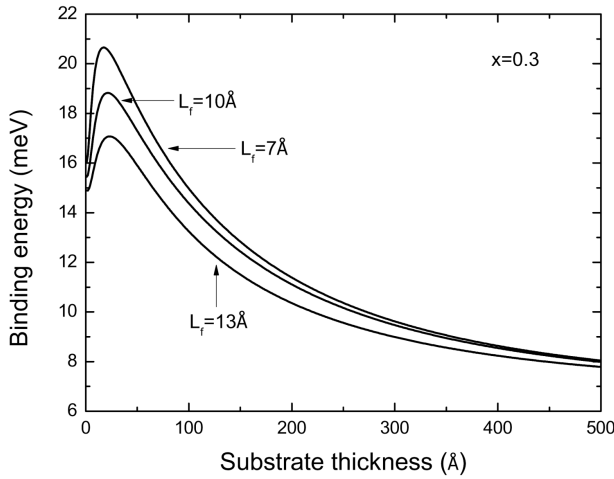
Fig. 3. The heavy-hole exciton binding energy in the GaAs film on $Al_{0.3}Ga_{0.7}As$ substrate as a function of the substrate thickness at different values of the film thickness $L_f = 7, 10, 13$ Å, respectively.

Fig. 5. The binding energy for the heavy-hole and light-hole excitons in the GaAs film on $Al_{0.3}Ga_{0.7}As$ substrate as a function of the substrate thickness at the film thickness $L_f = 10$ Å.
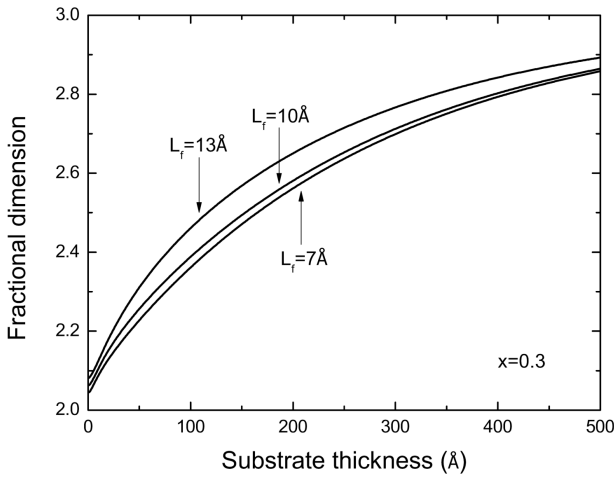

Fig. 4. The corresponding fractional dimension D as a function of the substrate thickness at different values of the film thickness $L_f = 7, 10, 13$ Å, respectively.

Fig. 6. The corresponding fractional dimension D for the heavy-hole and light-hole excitons as a function of the substrate thickness at the film thickness $L_f = 10$ Å.

The binding energy for the heavy-hole and light-hole excitons in the GaAs film on $Al_{0.3}Ga_{0.7}As$ substrate as a function of the substrate thickness is shown in Fig. 5, at the film thickness $L_f = 10$ Å. It is seen that the binding energies for the heavy-hole and light-hole excitons both exhibit their maxima with increase of the substrate thickness. The maxima appear at the film thicknesses $L_s \approx 21$ Å for heavy-hole exciton and $L_s \approx 24$ Å for light-hole exciton, respectively. We note that the heavy-hole exciton binding energy begins to decrease later than the light-hole one as the substrate thickness decreases. This is due to the z-direction effective masses. It also can be seen that, at a certain substrate thickness, the heavy-hole exciton binding energy is bigger than the light-hole one because of the ratio of the in-plane effective masses.

The fractional dimension D corresponding to the fractional-dimensional result in Fig. 5 is displayed in
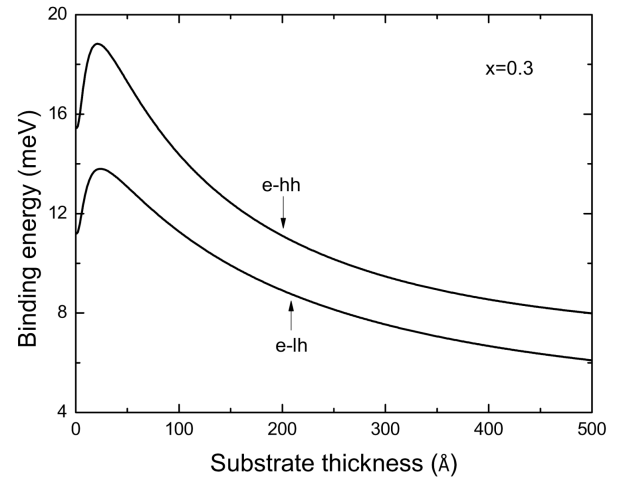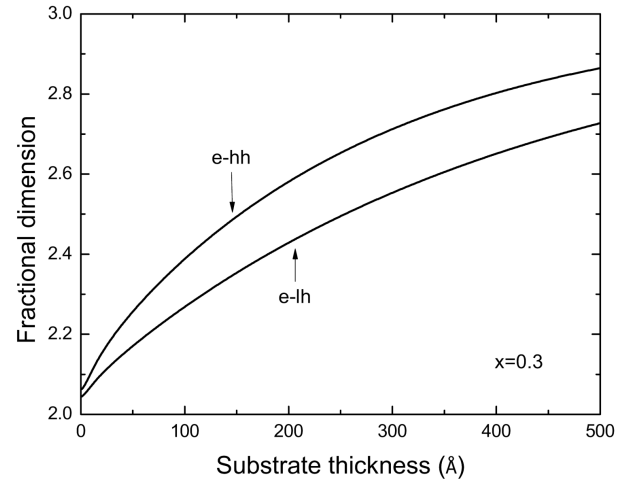
Fig. 6, as a function of the substrate thickness. For the case of heavy-hole and light-hole excitons, the fractional dimensions all increase monotonously as the substrate thickness increases. The values of the fractional dimension start from D $\approx$ 2.06 for heavy-hole exciton and D $\approx$ 2.04 for light-hole exciton, respectively. We note that the light-hole exciton fractional dimension is smaller than the heavy-hole one at a certain substrate thickness because of the ratio of the in-plane effective masses. We believe that the result is due to the fact that the light-hole exciton is more compressed by the system.

In order to understand the maxima of the exciton binding energies, we note that the exciton binding energy (see Eq. (3)) depends on two factors $(2/(D-1))^2$ and E_0^*. The former depends on the fractional dimension D of the GaAs film on $Al_xGa_{1-x}As$ substrate, and the latter is determined by the material parameters (see

Eqs. (4), (12), (13)). Although the fractional dimension increases monotonously, the exciton binding energy does not decrease monotonously. The exciton binding energy first increases and then decreases, exhibiting a maximum. The maximum in the exciton binding energy appear as a consequence of the combined influence between the fractional dimension and the material parameters.

4. Conclusions

The FDA have been used, in which the real anisotropic semiconductor system is mapped into an effective isotropic space with a fractional dimension, in the study of exciton binding energies in GaAs films on $Al_xGa_{1-x}As$ substrates. For different aluminum contents and film thicknesses, the exciton binding energies are obtained as functions of the substrate thickness. The numerical results shown that, for different aluminum contents and film thicknesses, the exciton binding energies in GaAs films on $Al_xGa_{1-x}As$ substrates all exhibit their maxima as the substrate thickness increases. It is also shown that the binding energies of heavy-hole and light-hole excitons both have their maxima as the substrate thickness increases. Moreover, the heavy-hole exciton binding energy is bigger than the light-hole one at a certain substrate thickness which is due to the ratio of the in-plane effective masses.

Acknowledgments

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