Fractional-dimensional approach for excitons in GaAs films on $Al_xGa_{1-x}As$ substrates*

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

Keywords: exciton binding energy, GaAs film, fractional-dimensional approach

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1. Introduction

In the last few decades, a large amount of work has been devoted to the research on the physics character 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 the potential applications in a wide range of electronic and optoelectronic devices. In fact, excitons have great effects on a variety of physical phenomena observed in these structures. Therefore understanding these properties such as the increase in the exciton binding energy due to the confinement of the carriers has become an important topic in the study of low-dimensional structures in the last few decades.

Since the pioneering work on exciton in a polar crystal by Haken,[1] a great deal of work has been devoted to study the excitonic properties in films theoretically and experimentally. Several authors calculated the binding energies of excitons in free-standing GaAs films by using variational schemes.[2] The optical spectroscopy of large-momentum excitons in GaAs films was experimentally and theoretically investigated by some researchers.[3,4] Photoluminescence (PL) spectrum measurements were used to study exciton[5,6] and exciton–polariton[7] problems and to determine the exciton binding energies[8,9] 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. As far as we know, there is not much work on the exciton properties in a GaAs film on an $Al_xGa_{1-x}As$ substrate.

Of particular interest to the present work is the fractional-dimensional approach (FDA) first proposed by He[10–13] to study excitons and optical properties of anisotropic solids. In this approach, the Schrödinger equation for a real anisotropic system is solved in a noninteger-dimensional space where the interactions are assumed to occur in an isotropic effective environment, and the essential quantity is the fractional dimension D associated with the effective medium and 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,[14–18] biexcitons,[19–21] magnetoexciton,[22–24] excitonic and impurity states,[23,25–30] polarons,[31–34] and exciton–phonon interaction[35–38] in anisotropic semiconductor heterostructures. However, to the best of our knowledge, the FDA has not been extended to investigate excitons in a GaAs film on an $Al_xGa_{1-x}As$ substrate.

In our preview work, we used the FDA to study the polaron effect in a GaAs film deposited on $Al_xGa_{1-x}As$ substrate.[39–41] 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 exciton + GaAs film system is realistically described by an equivalent isotropic hydrogenic system in a fractional D-dimensional space, a problem which can be solved analytically. As functions of the film thickness, the exciton binding energies are calculated. This paper is organized

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as follows. In Section 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 given in Section 3, and conclusions are given in Section 4.

2. Theoretical framework

Let us consider the problem of an exciton confined in a semiconductor GaAs film on $Al_xGa_{1-x}As$ substrate (growth axis along the z direction). Within the effective mass and the parabolic band approximations, the Hamiltonian for the exciton can be given by

$$H = -\frac{\hbar^2}{2m_{\rm e}(z_{\rm e})}\nabla_{\rm e}^2 - \frac{\hbar^2}{2m_{\rm h}(z_{\rm h})}\nabla_{\rm h}^2 - \frac{e^2}{\varepsilon|\boldsymbol{r}_{\rm e}-\boldsymbol{r}_{\rm h}|} + V_{\rm e}(z_{\rm e}) + V_{\rm h}(z_{\rm h}), \tag{1}$$

where $m_{\rm e}$ and $m_{\rm h}$ are the z-dependent (film or substrate) effective masses of electron and hole, respectively, and $V_{\rm e}$ and $V_{\rm h}$ are the confining potentials. For the case of no electron and hole escaping from the system, the potentials of the GaAs film on $Al_xGa_{1-x}As$ substrate are characterized by

$$V_j(z_j) = \begin{cases} V_{\rm f}(=0), & \text{if } 0 \le z_j \le L_{\rm f}, \\ V_{{\rm s}j}, & \text{if } L_{\rm f} < z_j < L_{\rm f}+L_{\rm s}, \\ \infty, & \text{otherwise}, \end{cases} \tag{2}$$

where $j = {\rm e}, {\rm h}$ represent the electron and the hole, respectively, $L_{\rm f}$ and $L_{\rm s}$ represent the film thickness and the substrate thickness, respectively, and subscripts f and s label the film (GaAs) and the substrate ($Al_xGa_{1-x}As$) regions, respectively. The z-dependent effective masses of electron and hole are characterized by

$$m_j(z_j) = \begin{cases} m_{{\rm f}j}, & \text{if } 0 \le z_j \le L_{\rm f}, \\ m_{{\rm s}j}, & \text{if } L_{\rm s} < z_j < L_{\rm f}+L_{\rm s}, \\ 0, & \text{otherwise}. \end{cases} \tag{3}$$

Using the FDA proposed by He,[10–13] 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 real system. By utilizing the Laplacian operator proposed by Stillinger,[42] who proposed axioms and operators for a noninteger-dimensional space, the discrete bound-state energies and orbital radii are given by

$$E_n = E_{\rm g} - \frac{E_0}{[n+(D-3)/2]^2}, \qquad a_n = a_0\left(n+\frac{D-3}{2}\right)^2, \tag{4}$$

where D is the dimension of a solid, $n = 1, 2, \ldots$ is the principal quantum number, and E_0 and a_0 are the effective Rydberg constant and the effective Bohr radius, respectively. Here $E_0 = (\varepsilon_0/\varepsilon)^2(\mu/m_0)R_{\rm H}$ and $a_0 = (\varepsilon/\varepsilon_0)(m_0/\mu)a_{\rm B}$, where $R_{\rm H}$ and $a_{\rm B}$ are the Rydberg constant and the Bohr radius, respectively, m_0 is the free-electron mass, and μ is the exciton reduced mass, $1/\mu = 1/m_{\rm e} + 1/m_{\rm h}$.

According to Eq. (4) 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

$$E_{\rm b} = \left(\frac{2}{D-1}\right)^2 E_0^*, \tag{5}$$

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

$$E_0^* = \left(\frac{\varepsilon_0}{\varepsilon^*}\right)^2\left(\frac{\mu^*}{m_0}\right)R_{\rm H}, \tag{6}$$

with ε^* being the mean value of the dielectric constant of GaAs film–$Al_xGa_{1-x}As$ substrate, and μ^* being the mean value of the exciton reduced mass. In Eq. (5), $D = 3, 2$, and 1 give respectively $E_{\rm b} = E_0^*, 4E_0^*$, and ∞, 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 the parabolic band approximations, the Hamiltonian for the single electron ($j = {\rm e}$) or hole ($j = {\rm h}$) can be given by

$$H_j = -\frac{\hbar^2}{2}\frac{\rm d}{{\rm d}z_j}\left(\frac{1}{m_j(z_j)}\frac{\rm d}{{\rm d}z_j}\right) + V_j(z_j). \tag{7}$$

The dimensional parameter D that guarantees the mapping of the real system into the fractional-dimensional space can be calculated through the relation[31]

$$D = 3 - \exp(-\xi), \tag{8}$$

where

$$\xi = \frac{\text{length of confinement}}{\text{effective characteristic length of interaction}}. \tag{9}$$

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 $L_{\rm f}^*$, which may be written as

$$L_{\rm f}^* = L_{\rm f} + \frac{1}{k_{\rm se}} + \frac{1}{k_{\rm sh}}, \tag{10}$$

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

$$k_{{\rm s}j} = \frac{\sqrt{2m_{{\rm s}j}(V_{{\rm s}j}-E_j)}}{\hbar}, \tag{11}$$

where E_j are the electron ($j = {\rm e}$) or hole ($j = {\rm h}$) eigenenergies determined by H_j (see Eq. (7)).

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

$$d_0^* = 2a_0^* = 2\frac{\varepsilon^*}{\varepsilon_0}\frac{m_0}{\mu^*}a_{\mathrm{B}}, \tag{12}$$

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

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

$$D = 3 - \exp\left(-\frac{L_{\mathrm{f}}^*}{2a_0^*}\right). \tag{13}$$

In the 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 the substrate materials should be considered. In order to take this fact into account, 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. [43]. In this way, they enter in the Hamiltonian of the system and weight the spatial integration with the square module of the electron ($j = \mathrm{e}$) and hole ($j = \mathrm{h}$) wave functions $\Psi_j(z_j)$ determined by H_j (Eq. (7)). Our effective fractional-dimensional exciton is then characterized by the following set of mean material parameters:

$$\left(m_j^*\right)^{-1} = \int_{-\infty}^{\infty} \frac{1}{m_j(z_j)} \left|\Psi_j(z_j)\right|^2 \mathrm{d}z_j, \tag{14}$$

$$\varepsilon^* = \int_{-\infty}^{\infty} \varepsilon(z) \left|\Psi(z)\right|^2 \mathrm{d}z. \tag{15}$$

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. (5), (6), and (13) with the mean values of the material parameters defined in Eqs. (14) and (15). We use the same set of material parameters as discussed by Smondyrev *et al.*[43] in our calculations. The numerical results are discussed in Section 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 film thickness is displayed in Fig. 1, for different Al concentrations at the substrate thickness $L_{\mathrm{s}} = 20$ Å. As can be seen, the exciton binding energy first increases as the film thickness decreases for different Al concentrations, as long as the exciton wave function remains confined in the film region. For thin films, the wave function starts to penetrate into the substrate and the exciton binding energy actually begins to decrease as the film thickness is reduced. Therefore, the exciton binding energies exhibit maxima at the film thicknesses $L_{\mathrm{f}} \approx 58$ Å for $x = 0.2$, $L_{\mathrm{f}} \approx 44$ Å for $x = 0.3$, and $L_{\mathrm{f}} \approx 35$ Å for $x = 0.4$. Notice that this behavior was also obtained in the case of excitons in GaAs–$Al_xGa_{1-x}As$ quantum wells by using the FDA.[14,18] It is also worthwhile noting that different Al concentrations have a significant influence on the exciton binding energy in thin and medium films, but have no significant influence in thick films. This behavior was also obtained in the case of excitons in GaAs–$Al_xGa_{1-x}As$ quantum wells by using the FDA.[14,18]

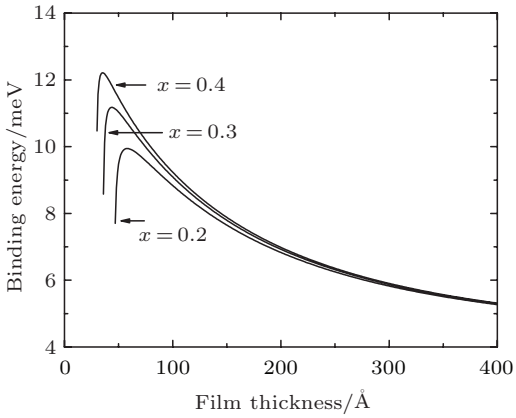


Fig. 1. The heavy-hole exciton binding energy in the GaAs film on $Al_xGa_{1-x}As$ substrate as a function of the film thickness for different Al concentrations at the substrate thickness $L_{\mathrm{s}} = 20$ Å.

The fractional dimension D corresponding to the fractional-dimensional result in Fig. 1 is shown in Fig. 2 as a function of the film thickness. With an extremely thick film, the system behaves as a GaAs bulk and consequently the fractional dimension approaches to the limit value $D = 3$. When the film thickness decreases, the system becomes more and more confined, the exciton becomes more compressed, and the effective dimension decreases, reaching minima at the film thicknesses $L_{\mathrm{f}} \approx 60$ Å for $x = 0.2$, $L_{\mathrm{f}} \approx 47$ Å for $x = 0.3$, and $L_{\mathrm{f}} \approx 39$ Å for $x = 0.4$. Notice that this behavior was also predicted in the case of excitons in GaAs-$Al_xGa_{1-x}As$ quantum wells within the FDA.[14,18] As the film thickness continues to decrease and is less than the exciton size, the exciton wave function starts to leak into the substrate so that the fractional dimension begins to increase. It is also worth remarking that different Al concentrations have a significant influence on the fractional dimension for thin and medium films, but have no significant influence for thick films. This behavior was also predicted in the case of excitons in GaAs-$Al_xGa_{1-x}As$ quantum wells within the FDA.[14,18]

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 film thickness is displayed in Fig. 3, for different substrate thicknesses $L_{\mathrm{s}} = 20$ Å, 50 Å, 100 Å. It can be seen that for different substrate thicknesses, the exciton binding energy has a maximum as the film thickness increases. The maxima appear at the film thicknesses $L_{\mathrm{f}} \approx 44$ Å, 35 Å, 31 Å, respectively. We note that the exciton binding energy increases with increasing

substrate thickness. This is due to the ratio of the GaAs film–$Al_xGa_{1-x}As$ substrate material parameters. It is also worth noting that different substrate thicknesses have a significant influence on the exciton binding energy for thin films but have no significant influence for thick films.

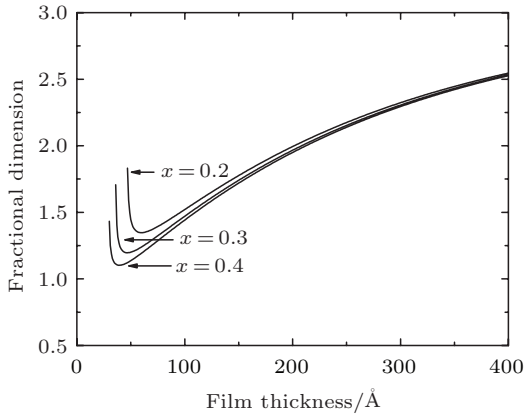


Fig. 2. The corresponding fractional dimension D as a function of the film thickness for different Al concentrations at the substrate thickness $L_s = 20$ Å.

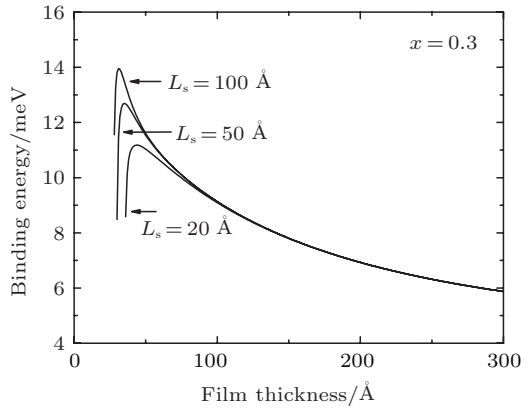


Fig. 3. The heavy-hole exciton binding energy in the GaAs film on $Al_{0.3}Ga_{0.7}As$ substrate as a function of the film thickness at different substrate thicknesses $L_s = 20$ Å, 50 Å, 100 Å.

The fractional dimension D corresponding to the fractional-dimensional result in Fig. 3 is shown in Fig. 4 as a function of the film thickness. For different substrate thicknesses, a structure with a minimum is obtained in the behavior of the fractional dimension. The minima appear at the film thicknesses $L_f \approx 47$ Å, 46 Å, 46 Å, respectively. It is also observed that, different substrate thicknesses significantly influence the fractional dimension for thin films but have no significant influence for thick films.

The binding energies 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 film thickness are displayed in Fig. 5, with the substrate thickness $L_s = 20$ Å. It is seen that the binding energies for the heavy-hole and light-hole excitons both exhibit their maxima with increasing film thickness. The maxima appear at the film thicknesses $L_f \approx 44$ Å for the heavy-hole exciton and $L_f \approx 50$ Å for the light-hole exciton. It is easily understood that the binding energies for the heavy-hole and light-hole excitons first increase as the film thickness decreases for the thicker film case, since the exciton wave function remains mainly confined in the film region. Once the film thickness is reduced and less than the exciton size, the exciton wave function will penetrate into the substrate region so that the binding energies decrease suddenly. We note that the heavy-hole exciton binding energy begins to decrease later than the light-hole one as the film thickness decreases. This is due to the z-direction effective masses. This behavior was also obtained by using the FDA in the case of excitons in GaAs-$Al_xGa_{1-x}As$ quantum wells.[14] It can also be seen that at a certain film thickness, the heavy-hole exciton binding energy is larger than the light-hole one because of the ratio of the in-plane effective masses. It is noteworthy that this result is quite different from the case of excitons in GaAs–$Al_xGa_{1-x}As$ quantum wells.[14] This should be due to the different definition of effective masses for the heavy-hole and light-hole excitons in Ref. [14]. In this paper, we use a consistent set of material parameters as discussed in Ref. [43].

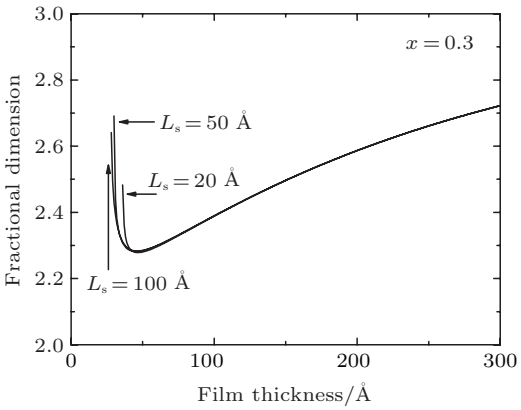


Fig. 4. The corresponding fractional dimension D as a function of the film thickness at different substrate thicknesses $L_s = 20$ Å, 50 Å, 100 Å.

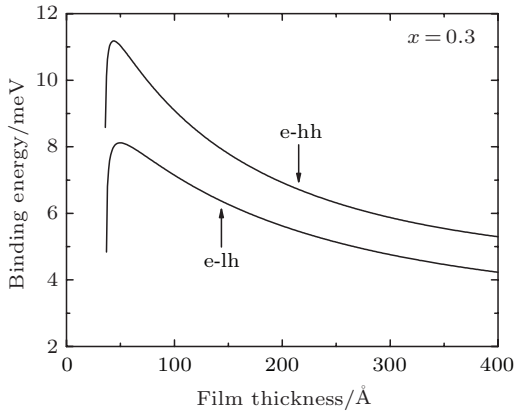


Fig. 5. The binding energy for the heavy-hole and light-hole excitons in the GaAs film on $Al_{0.3}Ga_{0.7}As$ substrate as a function of the film thickness at the substrate thickness $L_s = 20$ Å.

The fractional dimension D corresponding to the fractional-dimensional result in Fig. 5 is shown in Fig. 6 as a

function of the film thickness. For both heavy-hole and light-hole excitons, a structure with a minimum is predicted in the behavior of the fractional dimension. The minima appear at the film thicknesses $L_f \approx 47$ Å for the heavy-hole exciton and $L_f \approx 53$ Å for the light-hole exciton. On account of the z-direction effective masses, the heavy-hole exciton fractional dimension begins to increase later than the light-hole one as the film thickness decreases. We note that, for relatively thick films, the light-hole exciton fractional dimension is smaller than the heavy-hole one at a certain film thickness because of the ratio of the in-plane effective masses. The result for relatively thick films is due to the fact that the light-hole exciton is more compressed by the system.

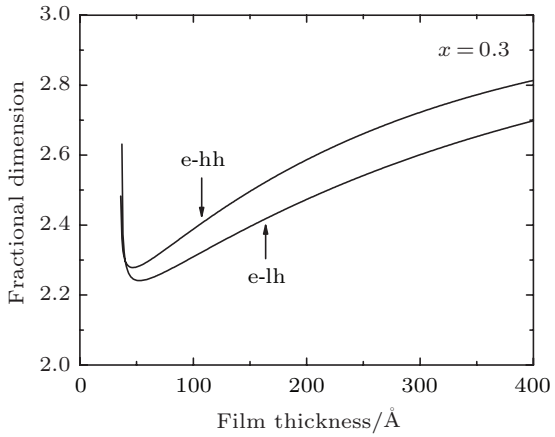


Fig. 6. The corresponding fractional dimension D for the heavy-hole and light-hole excitons as a function of the film thickness at the substrate thickness $L_s = 20$ Å.

4. Conclusion

We have used the FDA, in which the real anisotropic semiconductor system is mapped into an effective isotropic space with a fractional dimension, to study the exciton binding energies in GaAs films on $Al_xGa_{1-x}As$ substrates. For different aluminum concentrations and substrate thicknesses, the exciton binding energies are obtained as a function of the film thickness. The numerical results show that, for different aluminum concentrations and substrate thicknesses, the exciton binding energies in GaAs films on $Al_xGa_{1-x}As$ substrates all exhibit their maxima with increasing film thickness. It is also shown that the binding energies of heavy-hole and light-hole excitons both have their maxima with increasing film thickness. Moreover, the heavy-hole exciton binding energy is larger than the light-hole one at a certain film thickness, which is quite different from the case of excitons in GaAs-$Al_xGa_{1-x}As$ quantum wells.

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