Polaron effect influenced by thicknesses of GaAs film and Al\textsubscript{x}Ga\textsubscript{1-x}As substrate

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Abstract. The binding energy and effective mass of a polaron confined in a GaAs film deposited on Al\textsubscript{x}Ga\textsubscript{1-x}As substrate are studied theoretically within the framework of the fractional-dimensional approach and by using a correctional length of confinement. The numerical results for the polaron binding energy and effective mass in the GaAs film deposited on Al\textsubscript{x}Ga\textsubscript{1-x}As substrate are obtained as functions of the film thickness and substrate thickness. Through the correctional length of confinement, the problem of the original fractional-dimensional approach for the jumps of the polaron binding energy and mass shift with increasing the film thickness is solved. Our calculations show that the polaron binding energy and mass shift decreases monotonously as the film thickness increases. It is also shown that the polaron binding energy and mass shift both have their maxima as the substrate thickness increases.

1. Introduction

With the progress of semiconductor growth techniques, low-dimensional semiconductors can be prepared into various shapes. In particular, the GaAs film deposited on Al\textsubscript{x}Ga\textsubscript{1-x}As substrate is an important low-dimensional semiconductor. It is known that the electron–Longitudinal Optical (LO) phonon interaction leading to the polaron effect is observably influenced by the confinement which may strongly affect the optoelectronic and transport properties of these weak polar low-dimensional systems. Many theoretical models have been proposed by different researchers. However, most of the models have complex and lengthy calculations. We perform our study based on the fractional-dimensional approach proposed by He [1, 2]. In the fractional-dimensional approach, the anisotropic interactions in actual three-dimensional space are treated as isotropic ones in an effective fractional-dimensional space, which dimension is determined by the degree of anisotropy of the actual system. Therefore given this simple value—the dimension, the actual system can be modeled in a simple analytical way. In the past few years, the fractional-dimensional approach has been successfully used in studying exciton [3-7], magneto-exciton [8, 9], biexciton [10-12], impurity states [6, 13-20] in semiconductor microstructures and The electron–phonon effects on excitons in quantum well structures. Some researchers have used the fractional-dimensional approach to treat the polaron problems in sandwich structure GaAs-Al\textsubscript{x}Ga\textsubscript{1-x}As quantum wells, and obtained an easy estimation of
the polaron corrections with a good accuracy [21-28]. The polaron in a GaAs film, different from the polaron in the sandwich structure, is the research content of this paper.

We have studied the polaron [29-31] and exciton [32, 33] in a GaAs film deposited on Al$_x$Ga$_{1-x}$As substrate within the fractional-dimensional approach. In this paper, we correct the length of confinement and introduce the fractional-dimensional approach to the study of a polaron in a GaAs film deposited on Al$_x$Ga$_{1-x}$As substrate. The correctional length of confinement for a polaron in a GaAs film is determined and used in the fractional-dimensional approach. As functions of the film thickness and substrate thickness, the polaron binding energy and mass shift are calculated.

2. Fractional-dimensional approach

For a polaron in a GaAs film deposited on Al$_x$Ga$_{1-x}$As substrate and the case of no electron escaping from the structure, the potential of the structure is characterized by

\[
V(z) = \begin{cases} 
V_w &= 0 \quad \text{if} \quad 0 \leq z \leq L_w, \\
V_b &= \text{if} \quad L_w < z < L_w + L_b, \\
\infty &= \text{otherwise}, 
\end{cases}
\]

(1)

where $L_w$ and $L_b$ represent the film and substrate thickness, respectively. The subscripts $w$ and $b$ label the GaAs film and Al$_x$Ga$_{1-x}$As substrate regions, respectively.

In our GaAs–Al$_x$Ga$_{1-x}$As structure, the motion of the single electron is described by the Schrodinger equation

\[
\left[ \frac{\hbar^2}{2m(z)} \frac{d}{dz} \left( \frac{1}{m(z)} \frac{d}{dz} \right) + V(z) \right] \Psi = E \Psi,
\]

(2)

where $\hbar$ represents the reduced Planck constant and $m(z)$ represents the electron $z$-dependent effective mass

\[
m(z) = \begin{cases} 
m_w &= \text{if} \quad 0 \leq z \leq L_w, \\
m_b &= \text{if} \quad L_w < z < L_w + L_b, 
\end{cases}
\]

(3)

and $E$ represents the electron ground state energy in the GaAs–Al$_x$Ga$_{1-x}$As structure.

By using the fractional-dimensional approach, the electron self energy due to the electron–LO phonon interaction in the weak coupling approximation can be obtained within second-order perturbation theory [21-24], where the polaron binding energy was given by

\[
\Delta E = \alpha \hbar \omega_{LO} G_1(D)
\]

(4)

and the polaron effective mass by

\[
m^* = \frac{m}{1 - \alpha G_2(D)}.
\]

(5)

In equations (4) and (5), $\alpha$ is the Frohlich constant, $\omega_{LO}$ is the LO phonon limit frequency in the non-dispersive approximation, $D$ represents the dimension and $m$ is the electron effective mass. The $D$-dependent functions $G_1(D)$ and $G_2(D)$ are given by

\[
G_1(D) = \frac{\sqrt{\pi}}{2} \frac{\Gamma[(D-1)/2]}{\Gamma[D/2]}
\]

(6)

and
respectively. In equations (6) and (7) \( \Gamma (x) \) is the Gamma function.
The dimension \( D \) can be calculated through the relation [21-24]
\[
D = 3 - \exp \left[ -\xi \right],
\]
where
\[
\xi = \frac{\text{length of confinement}}{\text{effective characteristic length of interaction}}.
\]

The effective length that describes the electron–LO phonon interaction is the polaron diameter
\[
2R_p \quad (R_p = \sqrt{\hbar^2/2m\omega_{LO}} \text{ is the polaron radius}),
\]
and the length of confinement is described by the equivalent width of the structure that will be discussed in Section 3.

In a GaAs film deposited on Al\(_x\)Ga\(_{1-x}\)As substrate structure, the film material parameters are different from the ones in substrate region. In order to take account of this fact, we can assign to the fractional-dimensional space an average of the material parameters over the polaron positions. Then our fractional-dimensional electron–LO phonon interaction is described by the following set of mean parameters:

\[
m^{-1} = \sum_{i \in \text{w,b}} \frac{P_i}{m_i}, \quad (10)
\]

\[
\omega_{LO} = \sum_{i \in \text{w,b}} \omega_i P_i, \quad (11)
\]

\[
\alpha = \left[ \sum_{i \in \text{w,b}} \left( \frac{P_i \omega_i}{\omega_{LO}} \sqrt{\alpha_i \frac{m_i \omega_{LO}}{m_i \omega_i}} \right) \right]^2, \quad (12)
\]

\[
R_p = \left[ \sum_{i \in \text{w,b}} \left( \frac{P_i \omega_i}{\omega_{LO}} \sqrt{\frac{\alpha_i R_{pi}}{\alpha}} \right) \right]^2, \quad (13)
\]

\[
R_{pi} = \frac{\hbar}{\sqrt{2m_i \omega_i}}. \quad (14)
\]

In equations (10)-(13) \( \omega_i \) and \( \alpha_i \) represent the phonon frequencies and the Frohlich constants in different regions, and
\[
P_w = \int_0^{l_w} | \psi (z) |^2 dz, \quad (15)
\]

\[
P_b = 1 - P_w. \quad (16)
\]
indicate the probabilities of finding the single electron in the GaAs film and AlxGa1-xAs substrate regions, respectively. Then the binding energy and effective mass of a polaron in the GaAs film deposited on AlxGa1-xAs substrate can be calculated in a simple method from equations. (4), (5) and (8) within the material parameter mean values defined in equations (10)-(14).

3. Length of confinement of a polaron in a GaAs film on AlxGa1-xAs substrate

The dimension D is determined by equations. (8) and (9), form which one can see that the definition of the length of confinement has significant influence on the dimension D. In our previous work [27-29], the length of confinement was characterized by an effective film thickness and given by

\[ L'_w = L_w + \frac{1}{k_b} \]  \hspace{1cm} (17)

where \( k_b \) represent the electron wave vector in the substrate. After solving the Schrödinger equation (2), the value of \( k_b \) can be obtained from the relation

\[ k_b = \sqrt{\frac{2m_b (V_b - E)}{\hbar}} , \]  \hspace{1cm} (18)

and equation (8) reduces to

\[ D = 3 - \exp \left[ - \frac{L'_w}{2R_p} \right] . \]  \hspace{1cm} (19)

In this paper, we use the equivalent width of the structure to define the length of confinement for the polaron in a GaAs film deposited on AlxGa1-xAs substrate. In our GaAs–AlxGa1-xAs structure, we can define the equivalent width as follows: when the electron energy \( E \) [see equation (2)] in actual structure is equal to the electron energy in an infinite quantum well which width is equal to \( L'_w \). We define the equivalent width \( a \) as the length of confinement in actual structure. The equivalent width \( a \) can be calculated through the relation

\[ E = \frac{\hbar^2 \pi^2}{2mL'_w^2} . \]  \hspace{1cm} (20)

The electron eigenenergy \( E \) can be obtained by solving the Schrödinger equation (2). Then the corresponding well width which characterizes the length of confinement \( L'_w \) can be calculated from equation (18). It is straightforward to check the rationality of equation (18): If the height of the potential barrier \( V_b = 0 \) [see equation (1)], then the electron energy of the system is equal to the electron energy of an infinite quantum well which width is equal to \( L_w + L_b \). In this case, the length of confinement of the electron motion is equal to \( L_w + L_b \). While if the height of the potential barrier \( V_b \rightarrow \infty \), then the electron energy of the system is equal to the electron energy of an infinite quantum well which width is equal to \( L_w \). In this case, the length of confinement of the electron motion is also equal to \( L_w \). When the height of the potential barrier \( V_b \) is between 0 and infinity, the length of confinement \( L'_w \) is between \( L_w \) and \( L_w + L_b \). Notice that, the form of equation (18) is very similar to the eigenstate energy in the infinite quantum wells. It is due to the potential similarity of our GaAs film–AlxGa1-xAs substrate and the infinite quantum wells in the case of no electron escaping from the structure (see equation (1)).

4. Numerical results and discussion

Our calculations are performed within a consistent set of material parameters as discussed by Smondyrev et al. [34]. The polaron binding energy (solid line) as a function of film thickness in the
GaAs film deposited on Al$_{0.3}$Ga$_{0.7}$As substrate at substrate thickness $L_w = 20 \text{Å}$ is shown in figure 1. It is seen that the polaron binding energy starts from the value $\Delta E \approx 5.17 \text{meV}$ and decreases monotonously as the film thickness increases. For narrow film thicknesses, the binding energy decreases quickly. With increasing the film thickness, the binding energy decreases more and more slowly. Comparing our present results (solid line) with our previous calculations (dashed line) within the length of confinement given by equation (15) [28], one can see that for large film thicknesses good agreement is found. However, with decreasing the film thickness, the discrepancy between both calculations become obviously. From our previous results (dashed line) one can see that the binding energy appears to jump at the film thickness $L_w \approx 36 \text{Å}$, that is relate to the electron wave vector $k_s$ expressed by equation (16). From equation (16) one can see that when the electron eigenenergy $E$ is very close to the height of the potential barrier $V_b$, $k_s \to 0$ and $1/k_s \to \infty$. This will lead to the length of confinement becomes very large [see equation. (15)]. Thus the dimension $D$ appears to jump at the film thickness $L_w \approx 36 \text{Å}$ [see figure 3 (dashed line)]. Because of the jump of the dimension $D$, the binding energy occurs to a corresponding jump. However, in the range of the variation of the film thickness, the dimension $D$ of the system should not appear to jump. In order to solve this problem, we use the equivalent width of the structure to define the length of confinement [see equation (18)]. In this correctional length of confinement, the dimension $D$ of the system does not appear to jump [see figure 3 (solid line)]. Consequently, the binding energy dose not appear to jump [see figure 1 (solid line)]. This is a reasonable result.

A similar behavior for the film thickness dependence of the polaron effective mass (solid line) compared with our previous calculations (dashed line) [28] can be appreciated in figure 2, where the film thickness dependence of the mass shift $\Delta m = \Delta m/\Delta m_w$ is displayed. Notice that, $\Delta m$ represents the ratio of the mass shift ($\Delta m = m^* - m$) to that in the film material ($\Delta m_w = m_w^* - m_w$).

The fractional dimension (solid line) compared with our previous calculations (dashed line) [28] as a function of the film thickness corresponding to the fractional-dimensional results in figure 1 and 2 is plotted in figure 3. It is seen that the fractional dimension (solid line) starts from the value $D \approx 2.25$ and increases monotonously with increasing the film thickness. As the film thickness increases, the confinement becomes more and more weak and consequently the fractional dimension has the limit value $D = 3$.

The polaron binding energy and mass shift (solid line) compared with our previous calculations (dashed line) [29] as functions of the substrate thickness in the GaAs film deposited on Al$_{0.3}$Ga$_{0.7}$As substrate at film thickness $L_w = 10 \text{Å}$ are shown in figure 4 and 5. It is seen that the binding energy and mass shift (solid line) both have their maxima as the substrate thickness increases. One can appreciate in figure 4 and 5 that the quantitative discrepancy between our present results (solid line) and our previous calculations (dashed line) is obvious. From this point one can see that the definition of the length of confinement has significant influence on the fractional-dimensional polaron binding energy and mass shift. It is seen that for very large substrate thicknesses the binding energy and mass shift (solid line) are both nearly a constant.

The fractional dimension (solid line) compared with our previous calculations (dashed line) [29] corresponding to our results in figure 4 and 5 is displayed in figure 6 as a function of the substrate thickness. It is seen that the fractional dimension (solid line) starts from the value $D \approx 2.13$ and increases monotonously with increasing the substrate thickness. As the substrate thickness increases, the fractional dimension increases more and more slowly and for very large substrate thicknesses the fractional dimension is nearly a constant. This is because once the substrate thickness increases to the large region, the electron eigenenergy $E$ decreases very slowly as the substrate thickness increases. So that makes the length of confinement [see equation (18)] increases very slowly. Consequently, for
large substrate thicknesses the fractional dimension increases very slowly with increasing the substrate thickness.

It can be seen from the above figures, using the new defined length of confinement, the problem of the original fractional-dimensional approach for the jumps of the polaron binding energy and mass shift with increasing the film thickness have been solved. The polaron binding energy and mass decreased more slowly with increasing the substrate thickness than the original fractional-dimensional calculations. It can been seen that, using the new defined length of confinement, the polaron binding energy and mass shift are quite different from the original fractional-dimensional calculations. This is because of the structure of the GaAs film deposited on Al$_x$Ga$_{1-x}$As substrate is different from the GaAs-Al$_x$Ga$_{1-x}$As quantum wells. This leads to a difference in the form of the formula of the length of confinement.

**Figure 1.** The polaron binding energy as a function of the film thickness in the GaAs film deposited on Al$_{0.3}$Ga$_{0.7}$As substrate at the substrate thickness $L_s = 20\,\text{Å}$. Solid curves correspond to the present results by using a correctional length of confinement and the dashed line to the original fractional-dimensional calculations [28].

**Figure 2.** The polaron mass shift as a function of the film thickness in the GaAs film deposited on Al$_{0.3}$Ga$_{0.7}$As substrate at the substrate thickness $L_s = 20\,\text{Å}$.
Figure 3. The corresponding fractional dimension as a function of the film thickness for a polaron in a GaAs film deposited on the Al_{0.3}Ga_{0.7}As substrate at the substrate thickness $L_a = 20 \, \text{Å}$. 

Figure 4. The polaron binding energy as a function of the substrate thickness in the GaAs film deposited on Al_{0.3}Ga_{0.7}As substrate at the film thickness $L_a = 10 \, \text{Å}$. Solid curves correspond to the present results by using a correctional length of confinement and the dashed line to the original fractional-dimensional calculations [29].
Figure 5. The polaron mass shift as a function of the substrate thickness in the GaAs film deposited on $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ substrate at the film thickness $L_w = 10 \text{ Å}$. 

Figure 6. The corresponding fractional dimension as a function of the substrate thickness for a polaron in a GaAs film deposited on $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ substrate at the film thickness $L_w = 10 \text{ Å}$. 

5. Conclusions
In conclusion, we have introduced the fractional-dimensional approach to the study of a polaron in a GaAs film deposited on $\text{Al}_{x}\text{Ga}_{1-x}\text{As}$ substrate within a correctional length of confinement. Through the correctional length of confinement, the problem of the original fractional-dimensional approach for the jumps of the polaron binding energy and mass shift with increasing the film thickness have been solved. Our calculations show that the polaron binding energy and mass shift decreases monotonously as the film thickness increases. It is also shown that the polaron binding energy and mass shift both have their maxima as the substrate thickness increases. These results shown that the fractional-
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dimensional approach developed here is useable and reasonable in the study of the polaron effect in a GaAs film deposited on AlₓGa₁₋ₓAs substrate.