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Far-infrared absorption studies of Be acceptors in δ-doped GaAs/AlAs multiple quantum wells

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Abstract We report a far-infrared absorption study of internal transitions of shallow Be acceptors in both bulk GaAs and a series of δ-doped GaAs/AlAs multiple quantum well samples with well thicknesses of 20, 15 and 10 nm. Low temperature far-infrared absorption measurements clearly show three principal absorption lines due to transitions of Be-acceptor states from the ground state to the first three odd-parity excited states, respectively. Using a variational principle, the 2p-1s transition energies of quantum confined Be acceptors are calculated as a function of the well width. It is found that the theoretical calculation of the $2p_z \rightarrow 1s$ transitions is in good agreement with the D-like line experimental data.

Keywords: shallow acceptor impurities, δ-doped, GaAs/AlAs multiple quantum wells, far-infrared absorptions.

1 Introduction

Studies of the internal transition of quantum confined shallow impurities are currently attracting a great deal of attention for the physical phenomena they exhibit and their potential for a range of opto-electronic applications, such as far-infrared detectors and a solid state Terahertz laser[1−4]. Confinement of such impurities in quasi-two-dimensional GaAs/$Al_xGa_{1-x}As$ quantum wells allows the tuning of their levels in a controlled way. For device applications, it is desirable that the dipole-allowed 1s-2p transition can be tuned to be outside of the main longitudinal optical phonon bands of semiconductors.

In the GaAs, beryllium is an acceptor species commonly used in opto-electronic de vices, it is relatively stable with respect to diffusion and has a binding energy of 28 meV

in the bulk[5]. Furthermore, the use of δ doping avoids the extension of the impurity energy levels resulting from the distribution of the dopant atoms along the growth direction of the quantum wells. The electronic states and properties of the shallow acceptors in the GaAs/$Al_xGa_{1-x}As$ quantum wells are not understood as well as those of shallow donors as the valence band of bulk GaAs is fourfold degenerate and contains a cubic term that must be taken into account to describe the acceptor states. Reeder *et al*.[6] reported the first far-infrared transition study of the Be acceptor in GaAs/$Al_{0.3}Ga_{0.7}As$ quantum wells. To the present date, however, there are no reported calculations of the p-like acceptor states in quantum wells. Although initial calculations of acceptor states in a GaAs/$Al_xGa_{1-x}As$ quantum well were made by Masselink *et al*.[7], only the results of the subband energies and the acceptor states $1s_{3/2}\Gamma_8$ and $2s_{3/2}\Gamma_8$ in quantum wells have been reported. For the Be δ-doped GaAs/AlAs multiple-quantum wells with doping at the well center, there have been few reports of either experimental or theoretical work. However, this system is of especial interest as it represents the maximum possible confinement for the acceptor states in the valence band and thus the maximum possible tuning range for the 1s-2p transition of the acceptor.

In this paper we measure far-infrared absorption spectra at low temperature for shallow Be acceptors in both bulk GaAs and a series of GaAs/AlAs multiple quantum wells with Be δ-doped at the well center and the well thicknesses of 10, 15 and 20 nm. The 1s-2p acceptor transition energy is calculated using a variational method as a function of the quantum well width and compared with the experimental results.

2 Experiment and results

Investigated Be δ-doped GaAs/AlAs multiple quantum wells and GaAs:Be bulk samples were grown by molecular-beam epitaxy, on semi-insulating (100) GaAs substrates. The growth of layers was performed under exact stoichiometric condition using the technique of stoichiometric low-temperature growth[8], which ensures high quality optical materials even at relatively low growth temperatures. Under these conditions, the quantum well structures were grown at 550℃ and without interruptions at the quantum well interfaces, which ensured negligible diffusion of the Be δ layers. Each of quantum wells contained a 50 Å wide AlAs barrier layer, while every GaAs well layer was δ-doped at the well center with Be acceptor atoms. The GaAs:Be bulk sample was a single 1-μm-thick epilayer of GaAs with Be doped uniformly, as a limiting case and to provide a basis for understanding well the quantum well results. Table 1 shows the characteristics of the samples studied. For Fourier-transform infrared absorption experimental meas-

Table 1 Characteristics of the samples studied

Well width (Å)	Number of wells	Dopant concentration (cm^{-2})	Dopant position
100	200	5×10^{10}	center
150	50	2.5×10^{12}	center
200	100	5×10^{10}	center
Bulk	1	2×10^{16}	uniform

urements, each of samples was thinned, polished and wedged to approximately a 5° angle to suppress optical interference between the front and back faces.

Far-infrared absorption experiments were performed using a Fourier-transform spectrometer equipped with a tungsten light source and multilayer wide band beamsplitter. The investigated samples and the Si bolometer detector were placed into the cryostat with liquid helium. The absorption spectra, averaged over 800 runs, were obtained in a wavelength range from 40 to 300 cm^{-1} at 4.2 K.

The lowest acceptor states in bulk GaAs are identified as $1s_{3/2}\Gamma_8$, $2p_{3/2}\Gamma_8$, $2s_{3/2}\Gamma_8$, $2p_{5/2}\Gamma_8$, $2p_{5/2}\Gamma_7$ and $2p_{1/2}\Gamma_6$. When acceptors are introduced into the GaAs/$Al_xGa_{1-x}As$ quantum wells, the degeneracy of the valence band is lifted at the Γ point due to the quantum well potential which reduces the point group symmetry from T_d to D_{2d}. Therefore, the $1s_{3/2}\Gamma_8$ acceptor ground state and $2p_{3/2}\Gamma_8$, $2s_{3/2}\Gamma_8$ and $2p_{5/2}\Gamma_8$ excited states are split accordingly into $1s_{3/2}(\Gamma_6+\Gamma_7)$ and $2p_{3/2}(\Gamma_6+\Gamma_7)$, $2s_{3/2}(\Gamma_6+\Gamma_7)$, $2p_{5/2}(\Gamma_6+\Gamma_7)$, respectively. Fig. 1 shows far-infrared absorption spectra in the region from 120 to 240 cm^{-1} for the samples listed in Table 1. Three principal absorption lines, labeled G-like, D-like and C-like, are clearly observed consistent with the literatures, which correspond to acceptor state transitions from the ground state, $1s_{3/2}(\Gamma_6+\Gamma_7)$, to the first three excited odd-parity states, $2p_{3/2}(\Gamma_6+\Gamma_7)$, $2p_{5/2}(\Gamma_6+\Gamma_7)$ and $2p_{5/2}\Gamma_7$, respectively. For the GaAs:Be bulk sample, the G, D and C absorption lines are evident at 135, 167 and 183 cm^{-1} respectively, in good agreement with what have been reported in refs. [6,9]. No A absorp-

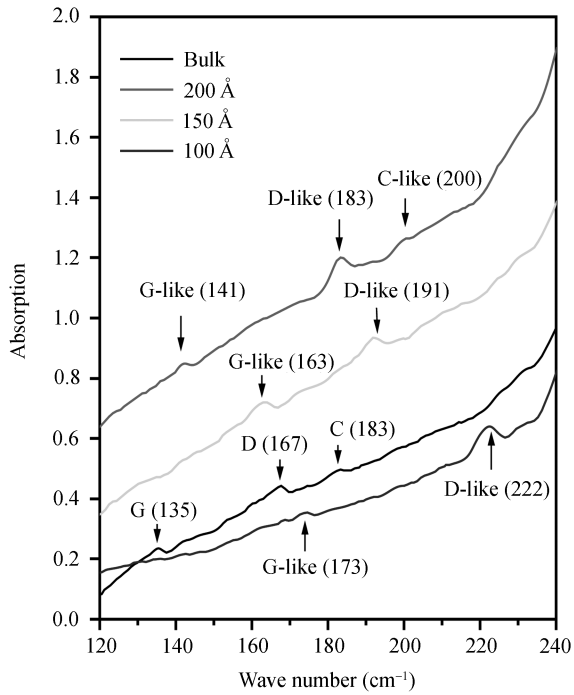

Fig. 1. Absorption spectra at 4.2 K of the GaAs:Be bulk and GaAs/AlAs multiple quantum wells samples with Be δ-doping at the well center and well width of 100, 150 and 200 Å.

tion line has been clearly observed, which arises from the transition between the $1s_{3/2}\Gamma_8$ ground state and the $2p_{3/2}\Gamma_6$ excited state. For the δ-doped multiple quantum wells samples, it can be easily seen that the G-like, D-like and C-like absorption lines all shift up in energy as the quantum well width decreases. This is due to the confinement effect of quantum wells pushing the hole closer to the negative core, thereby increasing Be acceptor binding energies[10]. Meanwhile, the ground state is lowered in energy relative to the excited states, resulting in an increase in transition energies with decreasing the quantum well width. This behavior is also similar to shallow donor impurities in GaAs/$Al_xGa_{1-x}As$ multiple quantum wells[2].

3 Calculation and discussion

3.1 Theory

The Hamiltonian of a beryllium impurity atom within a semiconductor GaAs/AlAs multiple quantum wells under the single-band effective mass and envelop function approximations is

$$H = -\frac{\hbar^2}{2}\frac{\partial}{\partial z}\frac{1}{m^*}\frac{\partial}{\partial z} + V(z) - \frac{e^2}{4\pi\varepsilon_0\varepsilon_r r}, \tag{1}$$

where m^* is the effective mass of a hole carrier, ε_r is the relative dielectric permittivity, $V(z)$ is the one-dimensional electrostatic potential and r is the distance between the impurity and the hole carrier. Placing the x and y origins on the impurity atom, which is at the position r_i, then

$$r^2 = x^2 + y^2 + (z - r_i)^2. \tag{2}$$

The success of variational approaches centers around the general choice of the trial wave function. We choose the produce of two terms as the trial wave function of a hole carrier:

$$\Psi = \psi(z)\phi(r), \tag{3}$$

where $\psi(z)$ is the wave function of the hole in the GaAs/AlAs multiple quantum wells without the acceptor impurity present and $\phi(r)$ is a hydrogenic like term describing the interaction between the hole and an acceptor ion.

The hydrogenic factor for the 1s ground state, $2p_x$ and $2p_z$ excited states is taken respectively as

$$\phi(r) = \exp\left(-\frac{r}{\lambda}\right) \quad \text{for the 1s state,} \tag{4}$$

$$\phi(r) = x\exp\left(-\frac{r}{\lambda}\right) \quad \text{for the } 2p_x \text{ state,} \tag{5}$$

$$\phi(r) = z\exp\left(-\frac{r}{\lambda}\right) \quad \text{for the } 2p_z \text{ state,} \tag{6}$$

where λ is well known as the Bohr radius, but now it is employed as a variational parameter.

The variational calculation is implemented by adjusting λ in order to minimize the

expectation value of the Hamiltonian operator. The total energy of the system is

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \tag{7}$$

The energy E is evaluated for different values of λ by direct numerical integration of the numerator and denominator in the above equation. For example,

$$\langle \Psi | H | \Psi \rangle = \int_0^\infty \mathrm{d}x \int_0^\infty \mathrm{d}y \int_0^\infty \Psi \left(-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m^*} \frac{\partial}{\partial z} + v(z) - \frac{e^2}{4\pi\varepsilon_0 \varepsilon_r r} \right) \Psi \mathrm{d}z. \tag{8}$$

These integrals are calculated using a simple strip summation over a three-dimensional uniform mesh, with the differentials in the kinetic energy component evaluated using finite difference expansions.

3.2 Results and discussion

In this subsection the numerical results of the energies of the $2p_x \rightarrow 1s$ and $2p_z \rightarrow 1s$ transitions of the Be acceptor at the center of the GaAs/AlAs multiple quantum wells as a function of the well width will be given. We use the formula $V(z) = 0.33\Delta E_g(x)$[11], where $\Delta E_g(x)$ is the difference in band gaps at $k = 0$ between GaAs and $Al_xGa_{1-x}As$. $\Delta E_g(x)$ is taken to $1247x$ meV and x is the mole fraction of the $Al_xGa_{1-x}As$ barriers. Although the single-well potential $V(z)$ makes it more appropriate for completely decoupled quantum wells, it will also be appropriate for multiple quantum wells with thick barriers that no hole wave function can penetrate. The effective mass m^* is used as the heavy-hole mass of $0.62m_0$, the typical value in bulk GaAs, where m_0 is the mass of an electron in the free space. The relative dielectric permittivity, ε_r, is set to 17.2. In previous theoretical calculations, a great deal of attention has been paid to the roles of the effective mass and the dielectric constant mismatches at interfaces in semiconductor hererostructures, and their effects on the shallow impurity energy levels in the quantum wells[12−14]. With m^* and ε_r parameters given above, we deduce the acceptor binding energy of 28.0 meV for very large well widths, which is in good agreement with the experimental result in bulk GaAs[5].

The two theoretical lines in Fig. 2 illustrate the energies of the $p_z \rightarrow 1s$ and $p_x \rightarrow 1s$ transitions calculated using the theory and parameters above described for the on-center Be δ-doped in GaAs/AlAs multiple quantum wells with a well width range from 50 to 300 Å. The solid circle dots and dot line show the experimental data of the D-like line transitions for all samples studied in Table 1. It can be seen that the theoretical calculation of the $p_z \rightarrow 1s$ transition is in good agreement with the experimental results. With the quantum-well width increasing, the theoretical calculation of the $p_z \rightarrow 1s$ transition tends towards the experimental result of the D-like line transition in the bulk GaAs:Be. It is suggested that the acceptors confined in GaAs/AlAs multiple quantum wells can be described as an ideal hydrogenic atom, and that the sing-band effective mass and envelope function approximation are reasonable. However, as the width of the quantum well decreases, the theoretical line of the $p_z \rightarrow 1s$ transition departs gradually from the experimental results measured. It is attributed to the potential spike resulting from the

monolayer of the δ-doped acceptors in GaAs/AlAs multiple quantum wells. The influence of the potential spike on acceptor states enhances, as the width of quantum wells decreases. In addition, the theoretical calculation of the $p_x \rightarrow 1s$ transition is close to the experimental results of the G-like absorption line measured, but it is not as good in agreement as the theoretical line of the $p_z \rightarrow 1s$ transition. Of course, there are some questions to be investigated further in our theoretical model, for example, the use of the dielectric constant in bulk GaAs has to be employed in the theoretical calculation for the GaAs/AlAs multiple quantum wells. In the majority of cases its use is probably fine, however, it is worthwhile noting that there is a change in the permittivity, as the effect of the quantum-well confinement on acceptor states enhances, and the bound hole approaches to the acceptor. In Fig. 1, the G-like, D-like and C-like energy positions are respectively slightly higher than those reported by Reeder *et al*.[6] for the same quantum well width but with $Al_{0.3}Ga_{0.7}As$ barriers, because of pure AlAs barriers with a stronger confinement effect on Be acceptors than $Al_{0.3}Ga_{0.7}As$ barriers.

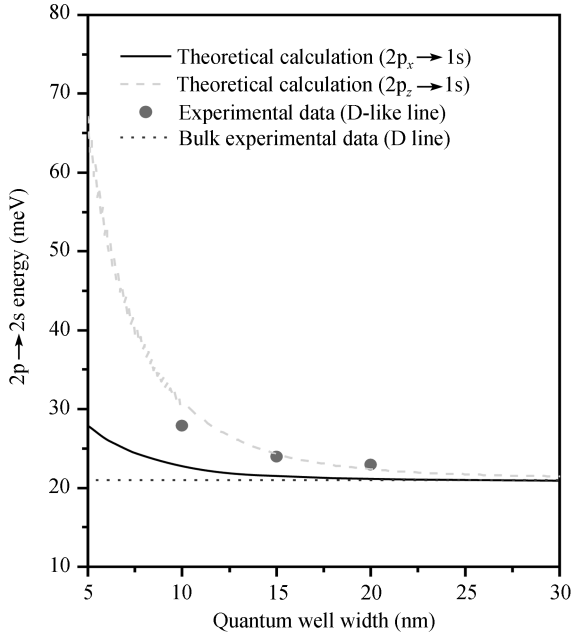

Fig. 2. Position of the D-like line as a function of well width (taken from Fig. 1). The solid line and dash line are the energies of the $2p_x \rightarrow 1s$ and $2p_z \rightarrow 1s$ transitions calculated with a variational method, respectively.

4 Conclusion

We have investigated experimentally far-infrared absorptions of the beryllium acceptors in the GaAs bulk and a series of GaAs/AlAs multiple quantum wells δ-doped with Be at the center of wells. The three principal absorption lines due to the 1s-2p transitions of the acceptors for all four samples are observed clearly. Using a variational method, the energies of the $2p_x \rightarrow 1s$ and $2p_z \rightarrow 1s$ transitions for the Be acceptors at the center of the

GaAs/AlAs multiple quantum wells have been calculated as a function of the well width. It is found that the theoretical calculation of the $2p_z \rightarrow 1s$ transition is in good agreement with the experiment results of the D-like line absorption.

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