Physics Letters A 373 (2009) 3490–3494

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Bound polaron in a wurtzite GaN/$Al_xGa_{1-x}N$ ellipsoidal finite-potential quantum dot

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ARTICLE INFO

Article history:
Received 9 April 2009
Received in revised form 12 June 2009
Accepted 20 July 2009
Available online 23 July 2009
Communicated by R. Wu

PACS:
73.21.La
71.38.-k
78.30.Fs

Keywords:
Quantum dots
Polaron
Electron–phonon interactions
Semiconductor

ABSTRACT

A variational method is used to study the ground state of a bound polaron in a weakly oblate wurtzite GaN/$Al_xGa_{1-x}N$ ellipsoidal quantum dot. The binding energy of the bound polaron is calculated by taking the electron couples with both branches of LO-like and TO-like phonons due to the anisotropic effect into account. The interaction between impurity and phonons has also been considered to obtain the binding energy of a bound polaron. The results show that the binding energy of bound polaron reaches a peak value as the quantum dot radius increases and then diminishes for the finite potential well. We found that the binding energy of bound polaron is reduced by the phonons effect on the impurity states, the contribution of LO-like phonon to the binding energy is dominant, the anisotropic angle and ellipticity influence on the binding energy are small.

1. Introduction

In recent years, the experimental techniques such as the molecular beam epitaxy (MBE) and metal-organic chemical vapor deposition (MOCVD) have led to the fabrication of many low dimensions semiconductor structures. One of the most significant achievements is the fabrication of zero-dimensional quantum dots (QDs) with well-controlled shape and size, and there has been much interest in investigating QDs both theoretically and experimentally due to their distinctive electronic and optical properties, which show a potential application in the electronic and optoelectronic devices [1,2]. Due to size quantization the physical properties of carriers in semiconductors QDs strictly depend on external shape of the object under investigation, the small change in external shape of quantum dot (QD) strongly influences energy spectrum and other physical properties. In the theoretical works, it is customary to assume a spherical shape for the QD [3,4]. Since deformation of spherical shape during QD growth is unavoidable, ellipsoidal shape represents a better approach to the actual problems [5–7], therefore theoretical studies on the ellipsoidal QD are needed. In most of the investigations, the height of the confinement potential of QD is infinite, to bring the problem closer to real situation, the finiteness of difference between potentials inside and outside the QD should be taken into account. Dvoyan [5] and Barati [8] made a research into the QD with ellipsoidal symmetry, they found that the binding energy of impurity state decreases with increasing ellipticity, but they have not considered the effects of optical phonons. Whereas the electron–phonon (e–p) interaction plays an important role in determining the physical properties of quantum dots (QDs) consisting of polar materials. The influence of e–p interaction could be enhanced due to the confinement of electron states [9].

Very recently, III-nitride (III-N) semiconductors have become important materials for the fabrication of optoelectronic devices operating in the green, blue, and ultraviolet spectral region [10–12]. In comparison to zinc-blende structure, the III-N semiconductors have the hexagonal wurtzite structure as their natural crystalline structure. As is well known, there are many more distinct phonon branches, and the phonon modes are not purely longitudinal or transverse except for the [0001] direction [13,14]. In bulk crystal the optical phonons are classified into the so-called ordinary and extraordinary modes, and all of them have been included in the study of e–p interaction [15]. A new Fröhlich e-p interaction Hamiltonian was put forward for the bulk case [16], within the non-retarded dielectric continuum model considering

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0375-9601/$ – see front matter
doi:10.1016/j.physleta.2009.07.053

only the three optical-phonon branches which are infrared active in this crystal structure. For wurtzite nitrides the dependence of the extraordinary optical phonon frequencies upon the phonon wave-vector $\vec{q}$ is not a function of the wave-vector magnitude but of the angle θ between $\vec{q}$ and the c-axis of the structure (referred as the z direction in the following). In a view of above-mentioned, it is very important and timely to investigate the influence of optical phonon in wurtzite nitride finite-potential QDs.

In the present Letter, taking the e–p and impurity–phonon (i–p) interactions into account, including both LO-like and TO-like phonon modes, we investigate the influences of phonons on an on-center hydrogenic impurity states in GaN/$Al_xGa_{1-x}N$ ellipsoidal QD by using a variational theory. The electronic confinement was modeled by a finite potential well. Our result seems to be more reliable than that obtained by other authors since the finite potential well and the interaction between the impurity and phonons have been taken into account.

This Letter is organized as follows: In Section 2, the binding energy of bound polaron and the polaronic shift for the binding energy in an ellipsoidal QD have been investigated by using Lee, Low and Pines (LLP)-like variational method [17]. Section 3 contains the numerical results and a detailed discussion. Finally, the conclusions are presented in Section 4.

2. Theory

Let us consider a semiconductor GaN ellipsoidal QD embedded in material $Al_xGa_{1-x}N$. The equation of the QD surface is

$$\frac{X^2+Y^2}{a^2}+\frac{Z^2}{c^2}=1 \quad (a<c), \tag{1}$$

where a and c are the semi-axes of the ellipsoid. The hydrogenic donor impurity is located at the center of the QD $(0,0,0)$. For wurtzite nitride semiconductor materials, we use Loudon model [14], take the c-axis along the z direction and denote it's perpendicular direction as $\perp$. The Hamiltonian of the electron-impurity system including the extraordinary LO-like and TO-like phonons and both the e–p and i–p coupling can be written as

$$H=H_{\rm e}+H_{\rm ph}+H_{\rm e,i-ph}. \tag{2}$$

The first term in Eq. (2) is electronic Hamiltonian and is written as

$$H_{\rm e}=\frac{p_\perp^2}{2m_\perp}+\frac{p_z^2}{2m_z}-\frac{e^2}{4\pi\varepsilon_0\varepsilon^\infty r}+U(\vec{r}), \tag{3}$$

where $m_\perp(m_z)$ is the effective mass perpendicular to (along) the c-axis, $U(\vec{r})$ is the confinement potential of ellipsoidal QD and r is the electron distance from the center, ε^∞ is the effective high-frequency dielectric constant and takes the form [18]

$$\frac{1}{\varepsilon^\infty}=\frac{\sin^2\alpha}{\varepsilon_\perp^\infty}+\frac{\cos^2\alpha}{\varepsilon_z^\infty}, \tag{4}$$

where α is the angle between $\vec{r}$ and the c-axis, $\varepsilon_\perp^\infty$ (ε_z^∞) is the high-frequency dielectric constant perpendicular to (along) the c-axis.

The second term in Eq. (2) is phonon Hamiltonian and is written as

$$H_{\rm ph}=\sum_{j\vec{q}}\hbar\omega_j a_{j\vec{q}}^+ a_{j\vec{q}}, \tag{5}$$

where $j(=L,T)$ is the mode-index of the phonon characteristic frequencies. $j=L$ stands for the LO-like phonon, $j=T$ stands for the TO-like phonon. The characteristic phonon frequencies of wurtzite structures satisfy the following conditions [15,16]:

$$\omega_L^2=\omega_{zL}^2\cos^2\theta+\omega_{\perp L}^2\sin^2\theta, \tag{6}$$

$$\omega_T^2=\omega_{zT}^2\sin^2\theta+\omega_{\perp T}^2\cos^2\theta, \tag{7}$$

where θ is the angle between the phonon wave-vector $\vec{q}$ and the c-axis.

The third term is the e–p and i–p interactions Hamiltonian and is written as

$$H_{\rm e,i-ph}=\sum_{j\vec{q}}\left[G_{j\vec{q}}\left(e^{i\vec{q}\cdot\vec{r}}-1\right)a_{j\vec{q}}+\text{h.c.}\right], \tag{8}$$

where "-1" term comes from the impurity localized at the origin, i.e. $r_{\rm ion}=0$ [19], and

$$G_{j\vec{q}}=\left(\frac{e^2\hbar}{\varepsilon_0 V}\right)^{1/2}\frac{1}{q}\left(\frac{\partial\varepsilon_\theta^j}{\partial\omega_j}\right)^{-1/2}, \tag{9}$$

$$\frac{\partial\varepsilon_\theta^j}{\partial\omega_j}=\frac{\partial\varepsilon_\perp(\omega_j)}{\partial\omega_j}\sin^2\theta+\frac{\partial\varepsilon_z(\omega_j)}{\partial\omega_j}\cos^2\theta. \tag{10}$$

We first carry out a unitary transformation to displace the equilibrium position of the ion

$$U_0=\exp\left[\sum_{j\vec{q}}\left(G_{j\vec{q}}^* a_{j\vec{q}}^+-G_{j\vec{q}}a_{j\vec{q}}\right)/\hbar\omega_j\right]. \tag{11}$$

The Hamiltonian (2) can be transformed into the following form

$$\begin{aligned}H^*&=U_0^{-1}HU_0\\&=\frac{p_\perp^2}{2m_\perp}+\frac{p_z^2}{2m_z}-\frac{e^2}{\varepsilon^* r}+U(\vec{r})+\sum_{j\vec{q}}\hbar\omega_j a_{j\vec{q}}^+ a_{j\vec{q}}\\&\quad+\sum_{j\vec{q}}\left(G_{j\vec{q}}e^{i\vec{q}\cdot\vec{r}}a_{j\vec{q}}+\text{h.c.}\right),\end{aligned} \tag{12}$$

where

$$\begin{aligned}\frac{1}{\varepsilon^*}&=\frac{1}{4\pi\varepsilon_0\varepsilon^\infty}-\frac{1}{2\pi^2\varepsilon_0}\\&\quad\times\sum_j\int\left(\omega_j\frac{\partial\varepsilon_\theta^j}{\partial\omega_j}\right)^{-1}r\sin\theta\cos(qr\cos\theta)\,d\theta\,dq.\end{aligned} \tag{13}$$

For convenience, we have dropped the infinite self-energy of a static point charge $-\sum_{j\vec{q}}|G_{j\vec{q}}|^2/\hbar\omega_j$.

For the sake of convenience, we give a further approximation of H^* by carrying out two unitary transformations as follows:

$$U_1=\exp\left[-i\sum_{j\vec{q}}a_{j\vec{q}}^+ a_{j\vec{q}}(\vec{q}_\perp\cdot\vec{\rho}+q_z z)\right], \tag{14a}$$

$$U_2=\exp\left\{\sum_{j\vec{q}}\left[a_{j\vec{q}}^+ f_j(\vec{q})-a_{j\vec{q}}f_j^*(\vec{q})\right]\right\}, \tag{14b}$$

where $f_j(\vec{q})$ and $f_j^*(\vec{q})$ are the variational functions and will be determined by minimizing the expectation value of the bound polaron energy. As a first approximation, we confined our discussion in the low-temperature limit, i.e., the phonon vacuum state $|0\rangle$ ($\langle 0|0\rangle=1$). After the two transformations the effective Hamiltonian for the bound polaron can be derived as

$$\begin{aligned}H_{\rm eff}&=\langle 0|U_2^{-1}U_1^{-1}H^*U_1U_2|0\rangle\\&=\frac{p_\perp^2}{2m_\perp}+\frac{p_z^2}{2m_z}+U(\vec{r})-\frac{e^2}{\varepsilon^* r}\\&\quad+\sum_{j\vec{q}}\left[G_{j\vec{q}}f_j(\vec{q})+G_{j\vec{q}}^* f_j^*(\vec{q})\right]\end{aligned}$$