Hydrostatic Pressure Effect of Binding Energy of Polarons in a GaAs/ AlxGa1-x As heterojunction

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Abstract : In a GaAs/ AlxGa1-x as heterojunction, the binding energy of bound polaron has been investigated. We find an increase in binding energy with an increase in hydrostatic pressure, almost linearly. The effect of the pressure is found more prominent when an impurity is located on the channel side. Valence bond offset varying with pressure was found. Variational method adopted for investigation.

I. Introduction

Over the last two decades, high pressure technology has become an effective tool to detect the physical properties of semiconductor materials and related low-dimensional systems, such as heterojunctions, quantum wells and superlattices. It has been attracting considerable attention both theoretically and experimentally.

Nakahara et. al.[1] studied the hydrostatic pressure dependence of the Raman spectra in Al_xGa_{1-x} As materials. Goni et. al.[2] investigated the direct and indirect optical-absorption edges for these kinds of ternarymixed crystals. the local vibration modes were given by Mc Cluskey et. al.[3] Reimannn et. al.[4] discussed the dependence of the band structure on pressure. It was found that the valence-band offset varying with pressure shows a dependence on the superlattice period. In order to investigate the property of phonons in depth, some authors studied experimentally the pressure effect of phonon energies by Raman scattering.[5] More recently, the hydrostatic pressure effect on the binding energies of donors in GaAs/Al_xGa_{1-x} As heterojunctions has been investigated.[6] The results show that the binding energies increase with pressure obviously, which qualitatively agrees with the results for excitons in quantum wells.[7]

II. Theory -

We consider a GaAs/Al_xGa_{1-x} As hetero junction whose channel side GaAs, denoted by material 1, is located at z > 0 and barrier side Al_xGa_{1-x} As, denoted by material 2, is located at z < 0, respectively. The interface of the heterojunction is defined as the *x-y* plane, which is assumed infinite without losing generality. In this system, a donor impurity, bearing a charge *e* is located at (0, 0, z_0) and interacts with a conduction electron bearing charge - *e* locating at (*x, y, z*). By considering the interaction from the LO and IO phonons, the Hamiltonian of this system can be written as

$$H = H_{x-y} + H_z + H_c + H_{ph} + H_{e,i-ph}$$ .... (1)

where

$$H_{x-y} = \frac{P_x^2 + P_y^2}{2m//1}\theta(z) + \frac{P_x^2 + P_y^2}{2m//2}\theta(-z)$$ .... (2)

$$H_z = \frac{P_z^2}{2m_{\perp 1}}\theta(z) + \frac{P_z^2}{2m_{\perp 2}}\theta(-z) + V(z) + \frac{e^2(\varepsilon_{\infty 1} - \varepsilon_{\infty 2})}{4z\varepsilon_{eff}(\varepsilon_{\infty 1} + \varepsilon_{\infty 2})}$$ .... (3)

$$H_c = -\frac{e^2}{\varepsilon(z, z_0)\left[x^2 + y^2 + (z - z_0)^2\right]^{1/2}}$$ .... (4)

$$H_{ph} = \sum_{k_1} hw_{L1} a_{k_1}^+ a_{k_1} \theta(z) = \sum_{k_2} hw_{L2} a_{k_2}^+ a_{k_2} \theta(-z) = \sum_{q,a} hw_a b_{q,a}^+ b_{q,a} \qquad \text{......................... (5)}$$

and

$$H_{e,i-ph} = \sum_k \left\{ \left[\frac{1}{k} \sum_\lambda B_\lambda(z) \sin(k_z |z|) e^{-i(k//\rho)} - B_{\lambda'}(z_0) \sin(k_z |z_0|) \right] a_k^+ + h.c. \right\}$$

$$+ \sum_{q,a} \left\{ \left[\frac{G_a}{\sqrt{q}} \left(e^{-i(q.\rho)} e^{-q|z|} - e^{-q|z_0|} \right) \right] b_{q,a}^+ + h.c. \right\} \qquad \text{....................... (6)}$$

All of the parameters used in the above equations were defined in a previous work.[8]

For the ground state of this system, the variational trial wave function is chosen as

$$|\Psi\rangle = |\phi(x,y)\rangle |\zeta(z)\rangle |0\rangle = |\phi(\rho)\rangle |\zeta(z)\rangle \prod_{k_{qa}} |0_k\rangle |0_{qa}\rangle \qquad \text{......................... (7)}$$

where

$$|\phi(\rho)\rangle = \left[\frac{1}{2\pi} \right]^{1/2} \gamma e^{ik//-\rho e-\gamma\rho/2} \qquad \text{....................... (8)}$$

$$\zeta(z) = \begin{cases} \zeta_A(z) = Bb^{1/2}(bz+\beta)e^{-bz/2} \\ \zeta_B(z) = B'b'^{1/2} e^{b'z/2} \end{cases} \qquad \text{....................... (9)}$$

where $\rho = \sqrt{x^2 + y^2}$ is the radial component of the electron coordinate in the *x*-*y* plane and $k_{//} = (k_x, k_y, 0)$. γ, b and b' are the independent variational parameters. In Eq. (7), $|0\rangle$ is the phonon-vacuum state. B and B' can be obtained by the continuity conditions of the wave functions and t heir first-order differentials at z = 0. In Eq. (8), the introduction of factor $e^{ik//\cdot\rho}$ is to recover the free polaron case when γ approaches 0.

To simplify the calculation for the *e - p* interaction we firstly carry out two 2D LLP-like transformations on the Hamiltonian as follows[8,9].

$$U_1 = \exp\left[\frac{i}{h} \left(P_{//} - h \sum_k k_{//} a_k^+ ak - h \sum_{q,a} q b_{q,a}^+ b_{q,a} \right) \cdot \rho \right] \qquad \text{....................... (10)}$$

$$U_2 = \exp\left[\sum_k \left(f_k a_k^+ - f_k^* ak \right) + \sum_{q,a} \left(g_{q,a} b_{q,a}^+ - g_{q,a}^* b_{q,a} \right) \right] \qquad \text{....................... (11)}$$

where f_k, $g_{q,a}$ and their complex conjugates are variational parameters. By using Eq. (7), we obtain the variational expectation energy of the bound polaron in the ground state :

$$E(b,b',\gamma) = \langle \Psi | U_2^{-1} U_1^{-1} H U_1 U_2 | \Psi \rangle$$

$$= E_a + \langle T \rangle + \langle V_d \rangle + \langle V_s \rangle + \langle V_0 \rangle + E_{image} + E_C - E_{LO} - \sum_a E_{Ia} \qquad \text{....................... (12)}$$

where the qualities of *E* were given in Ref. 8.

We minimize Eq. (12) with respect to γ, *b* and *b'* simultaneously to obtain the ground state energy E_{bq} for a bound polaron. Choosing $H_c = 0$ in Eq. (1) and using the same process, the ground state energy E_{fg} for a free polaron can be also derived. The binding energy of the bound polaron in the ground state can be written as

$$E_B = E_{fp} - E_{bp} \qquad \text{.................... (13)}$$

III. Results and Discussion

For a GaAs/Al$_x$Ga$_{1-x}$As heterojunction, the band mass of the electron has been considered as isotropic : $m_\perp = m_{//}$. We only consider the Al concentration for $x \leq 0.4$ and the pressure effect ranging from 0 to 40 kbar, for which Al$_x$Ga$_{1-x}$As is a direct band-gap semiconductor.

For a given Al concentration $x = 0.3$, impurity position $z_0 = 30$ A and areal electronic density $n_8 = 4.0 \times 10^{11}$/cm^2 and 8.0×10^{11}/cm^2 respectively, the binding energy of a bound polaron as a function of P is given by Fig. 1(a). It is found that E_B increases near linearly with pressure and the influence of pressure is weaker when the areal electronic density is larger. E_B increases 16.5% and 15.3%, whereas the net increase is 1.89 meV and 2.03 meV corresponding to $n_8 = 4.0 \times 10^{11}$/cm^2 and 8.0×10^{11}/cm^2, respectively by comparing the results at $P = 40$ kbar with that at $P = 0$ kbar.

In order to understand the pressure effect on the heterojunction systems, we also claculated the average distance $\langle z \rangle = B^2 \left(b + 4\beta + \beta^2 \right) / b = B'^2 / b'$ between the electron and the interface and the average distance $\langle \rho \rangle = 2 / \gamma$ between the electron and the impurity in the x-y plane. Figure 1(b) gives $\langle z \rangle$ and $\langle \rho \rangle$ as a function of pressure. It can be seen that the two average distances decrease with pressure and the pressure influence on $\langle \rho \rangle$ is more obvious. All of the results are consistent qualitatively with that without considering the effect of phonons.[6]

For the LO phonon mode, the phonon contribution to E_B is defined as

$$\Delta E_{LO} = -E_{LO} \left(free\ polaron \right) + E_{LO} \left(bound\ polaron \right) \quad\quad .... (14)$$

and for the IO phonon modes, the contribution is :

$$\Delta E_{I\sigma} = -E_{I\sigma} \left(free\ polaron \right) + E_{I\sigma} \left(bound\ polaron \right) \left(\sigma = \pm \right) \quad\quad .... (15)$$

where $\sigma = +, -$ corresponds to the IO phonon modes with higher and lower frequencies, respectively. From Fig. 1(c), one can see that $|\Delta E_{I-}|$, $|\Delta E_{I+}|$ and $|\Delta E_{LO}|$ also increase near linearly with pressure. For a given areal electronic density $n_8 = 4.0 \times 10^{11}$/cm^2 ($n_8 = 8.0 \times 10^{11}$/cm^2),, the pressure influence on $|\Delta E_{LO}|$ is strongest, which is 18.3% (16.3%) whereas the net increase is 0.0549 meV (0.0579 meV). On the other hand, the influence on $|\Delta E_{I-}|$ is stronger, which is 7.14% (7.77%) whereas the net increase is 0.010 meV (0.0132 meV). The influence on $|\Delta E_{I+}|$ is weakest.

For the given areal electronic density $n_8 = 4.0 \times 10^{11}$/cm^2, Al concentration $x = 0.3$ and pressure $P = 0$ kbar, 20 kbar and 40 kbar, respectively, E_B, $\langle z \rangle$, $\langle \rho \rangle$ and the phonon contribution to E_B varying with impurity position are calculated in Fig.2. The change of E_B is due to the com petition among the potential barrier V_0, the energy band bending and the attraction of the impurity, all of which are influenced by the pressure. E_B first increases then decreases with increasing z_0, mainly because the competition of the interface potential is weakened and the competition of conduction band bending is strengthened gradually - these induce the electron to move towards the interface. From Fig. 2(a) we can find that the following figures.
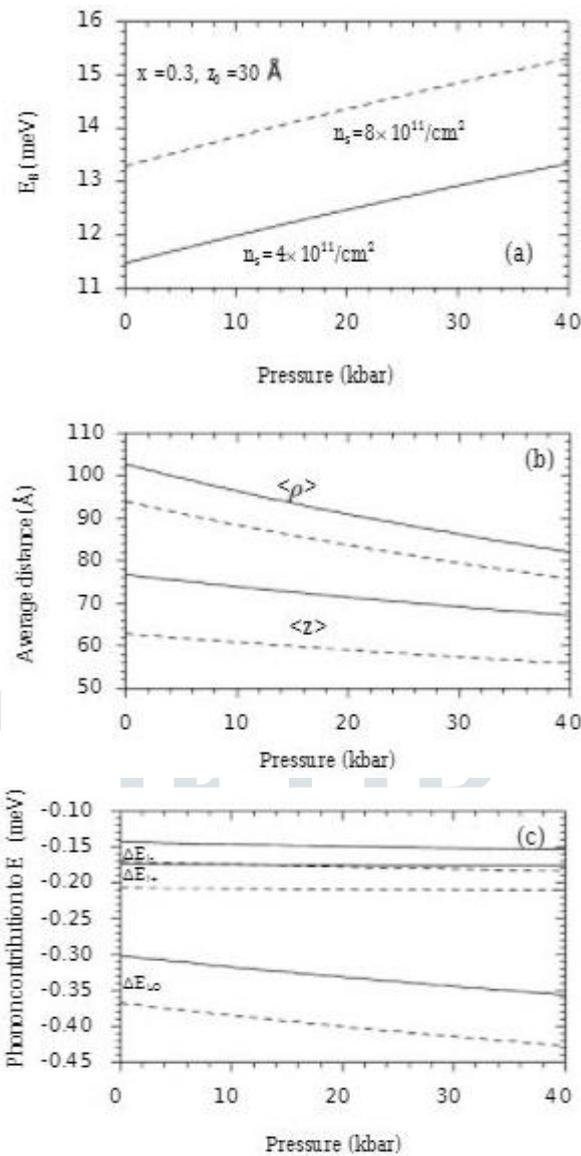
Fig.1 : For given areal electron densities (n8 = 4 × 1011/cm2 solid curves), 8 × 1011/cm2 (dashed curves), the calculated quantities as functions of pressure, in units of kbar, corresponding to the Al concentration x = 0.3 and impurity position z0 = 30 A are presented. (a) The binding energy EB in units of meV, (b) the average distance between t he electron and impurity in the x-y plane $\langle \rho \rangle$ and the distance between the electron and the interface $\langle z \rangle$ in units of A, (c) phonon contribution to EB, in units of meV. ΔE_{I+}, ΔE_{I-} and ΔE_{LO} are the results from the IO phonon modes with higher, lower frequencies and the LO phonon modes, respectively.

IV. Acknowledgement :

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