*J. Nano- Electron. Phys.*
**3** (2011) No1, P. 1041-1047

© 2011 SumDU
(Sumy State University)

PACS numbers: 73.21.La, 71.55 − i, 73.61.Ey, 71.30. + h.

# SIMULTANEOUS EFFECTS OF HYDROSTATIC PRESSURE AND GEOMETRY ON METAL-INSULATOR TRANSITION IN A CUBICAL QUANTUM DOT

***S. Rajashabala***[1], ***R. Kannan***[2]

[1] School of Physics, Madurai Kamaraj University,
palkalainagar,Madurai-625021,Tamilnadu,India.
E-mail: rajashabala@yahoo.com

[2] Department of Physics, Anna University of Technology Madurai,
Dindigul Campus, Dindigul-624622, India

*The ionization energies of a hydrogenic donor in a* GaAs- $Ga_{1-x}Al_xAs$ *cubical quantum dot system are obtained for various cross-sectional geometries. We have investigated the metal -insulator transition in such a system by considering the simultaneous effects of pressure and geometry. It is observed that, the ionization energies are increased due the geometry effect. Consecutively, the metal insulator transition couldn't occur for lower concentration of donor impurities. We present the results for infinite confinement.*

***Keywords:*** *HYDROGENIC DONOR, DONOR BINDING ENERGY, METAL-INSULATOR TRANSITION, QUANTUM DOT AND CROSS- SECTIONAL GEOMETRY.*

*(Received 04 February 2011 )*

## 1. INTRODUCTION

In the last few decades, there has been considerable interest in the study of impurity states in low dimensional quantum well systems due to their impending applications in electronic and optoelectronic devices [1-3]. The binding energy of shallow donor impurities in nanoscopic systems depends on materials, geometry, size and shape [4, 5]. The position of the impurity has a strong influence [6]. Schweizer et al. [7] have produced rectangular transversal section GaAs-(Ga, Al)As quantum well wires and quantum dots. The more real zero dimensional quantum hetero structure (cubic dot) was studied by Ribeiro and Latgre [8]. Oyoko et al. [9] studied donor impurities in a parallelepiped-shaped GaAs-(Ga, Al)As quantum dot. Kasapoglu et al. have studied the geometrical effects on shallow donor impurities in quantum well wire [10]. Jeyakumar et al. have investigated the effect of geometry on diamagnetic susceptibility of a hydrogenic donor in GaAs-(Ga, Al)As systems[11].

Doping in quantum dots (Qdots) plays a vital role when Qdots are used for various technological applications such as optoelectronic, magnetic, biological and spintronic applications. Optical properties of Qdots can be varied by changing the amounts [12] and the positions [13] of dopants in the Qdots. In the last few years, theoretical investigations on MIT in GaAs-$Ga_{1-x}Al_xAs$ quantum wells have been reported by several investigators. The purpose of the present work is to see, how the metal insulator transition (MIT) may affect due to the geometrical effect and pressure. Within our knowledge, the

influence of simultaneous effects of hydrostatic pressure and geometry on the MIT in a GaAs cubical quantum dot has not been reported.

This paper has been organized as follows. In Section2, the model and calculations is described. The Results and discussion is given in Section 3. Finally, a brief conclusion is given in Section 4.

## 2. MODEL AND CALCULATIONS

The Hamiltonian for a screened donor impurity in a GaAs cubical quantum dot is given by

$$H = \frac{-\hbar^2\nabla^2}{2m^*} - \frac{e^2}{\varepsilon(r)r} + V_D(r) \tag{1}$$

where $m^*$ is the effective mass of the donor electron in GaAs dot and $\varepsilon(r)$ is the dielectric screening function. The second term in Eqn.(1) which is responsible for the phase transition. We assume Thomas-Fermi dielectric screening function, which can be written as

$$\frac{1}{\varepsilon(r)} = \frac{e^{-\lambda r}}{\varepsilon} \tag{2}$$

Here $\lambda$ is screening parameter, which is related with density of states $[n(\xi)]$ at Fermi energy is given by,

$$\lambda^2 = \frac{4\pi e^2 n(\xi)}{\varepsilon} \tag{3}$$

The third term in Eqn.(1) which confines the donor electron within the quantum dot. The confining potential is given by

$$V_D(r) = \begin{cases} 0 & |x| \le \frac{R_x}{2}, |y| \le \frac{R_y}{2}, |z| \le \frac{R_z}{2} \\ \infty & \text{otherwise} \end{cases} \tag{4}$$

Here $R_x$, $R_y$ and $R_z$ give the dimension of the system along $x$, $y$ and $z$ axes. The ground state wave function for Hamiltonian (H) can be written as

$$\psi = \begin{cases} N\cos\left(\frac{\pi x}{R_x}\right)\cos\left(\frac{\pi y}{R_y}\right)\cos\left(\frac{\pi z}{R_z}\right)e^{-\alpha\sqrt{x^2+y^2+z^2}} & |x| \le \frac{R_x}{2}, |y| \le \frac{R_y}{2}, |z| \le \frac{R_z}{2} \\ 0 & \text{otherwise} \end{cases} \tag{5}$$

where $N$ is the normalization constant and $\alpha$ is the variational parameter. The Schrodinger equation is solved by variational method and the $\langle H \rangle$ can be written as

$$\langle H \rangle = \langle T \rangle + \langle V \rangle + \langle V_D(r) \rangle \tag{6}$$

where $\langle T \rangle$ is the expectation of kinetic energy which can be written as,

$$\langle T\rangle = \frac{-8N^2(\alpha)}{2*0.067}\int_0^{\frac{R_x}{2}}\int_0^{\frac{R_y}{2}}\int_0^{\frac{R_z}{2}}\psi\nabla^2\psi\,dxdydz \tag{7}$$

The expectation of impurity potential energy is given by

$$\left\langle V_D(r)\right\rangle = \frac{-8N^2(\alpha)}{12.65}\int_0^{\frac{R_x}{2}}\int_0^{\frac{R_y}{2}}\int_0^{\frac{R_z}{2}}\frac{\psi\nabla^2\psi}{\sqrt{x^2+y^2+z^2}}dxdydz \tag{8}$$

The expectation of confining potential energy is $\langle V_D(r)\rangle = 0$. To obtain the ionization energy, $H$ is minimized with respect to $\alpha$ and is calculated by using the following formula.

$$E_{ion} = E_{sub} - \left\langle H_{\min}\right\rangle \tag{9}$$

where $E_{sub}$ is the sub band energy which is calculated from the following formula for different dot geometries.

$$E_{sub} = \frac{\hbar^2}{2m*}\left[\left(\frac{\pi}{R_x}\right)^2 + \left(\frac{\pi}{R_y}\right)^2 + \left(\frac{\pi}{R_z}\right)^2\right] \tag{10}$$

### 2.1 Effect of hydrostatic pressure

Application of hydrostatic pressure modifies dot size, dielectric constant and effective mass in the following way [14].

$$R = R_0(1 - 2.6694\cdot 10^{-4}P)\,,\ \ \varepsilon(P) = 12.65 - 0.088P\,,\ \ m^*(P) = m^*(0)\exp(0.078P)\,,$$

where $P$ is expressed in GPa.
Using these variations the binding energy and the donor ionization energies of dot were obtained for 30 Kbar pressure using the variational method as explained above.

The effect of the diamagnetic susceptibility ($\chi_{dia}$) of a hydrogenic donor is calculated by using the following formula [15].

$$\chi_{dia} = \frac{-e^2}{6m^*\varepsilon c^2}\left\langle r^2\right\rangle$$

where $c$ is the velocity of light (which is equal to 137au and $e = 1$ in atomic units), and $\langle r^2\rangle$ is the mean square distance of donor electron from the donor ion. By making use of previous results the $\chi_{dia}$ values for an infinite cubical quantum dot are estimated. For infinite barrier model we use the expression,

$$\chi_{dia} = \frac{-8N^2(\alpha)}{6m^*\varepsilon c^2}\int_0^{\frac{R_x}{2}}\int_0^{\frac{R_y}{2}}\int_0^{\frac{R_z}{2}}\psi r^2\psi\,dxdydz \tag{11}$$

## 3. RESULTS AND DISCUSSION

The results obtained are shown in Figs. 1-4. The ionization energies of a hydrogenic donor in a cubical quantum dot for two different geometries such as $G_1(R_x, R_y, R_z)$ and $G_2(R_x, 0.5R_y, R_z)$ are presented in Fig. 1. It is noticed that the donor ionization energy increases when the dimension of the system along y axis ($R_y$) is reduced by half. This is mainly due to the compression of wave function. Also the donor ionization energy decreases as the dot size increases. This type of variation is common to all quantum well systems with infinite barriers [16].

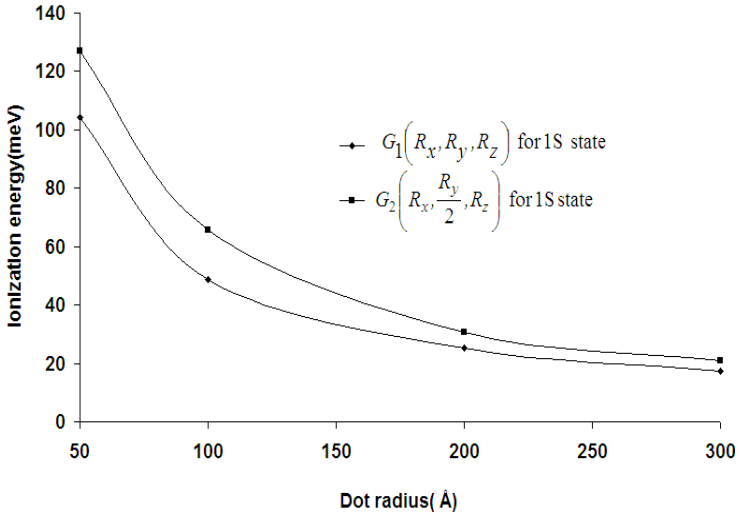



***Fig. 1*** *– Variation of ionization energy with radius for two different geometries*

The variation of ionization energy with donor impurity concentration is shown in Fig. 2 for an infinite cubical quantum dot with three different cross- sectional geometries namely $G_1(R_x, R_y, R_z)$, $G_2(R_x, 0.5R_y, R_z)$ and $G_3(R_x, 0.25R_y, R_z)$.Here the $R$ is taken as 200 Å. The ionization energy increases as the impurity concentration decreases. MIT (ionization energy goes to zero) takes place very quickly when there is no geometrical effect is included. It is concluded that as such the inclusion of geometrical effect has no vital role in the studies of MIT.

The variation of ionization energy with donor concentration in the presence of simultaneous effects of pressure and geometry on a cubical quantum dot is shown in Fig. 3. In this case, the cubical quantum dot may shrink due to application of pressure and geometry effect. It is reflected in the estimation of binding energy and in turn affects MIT of a cubical quantum dot. It is noted that, the ionization energy is almost constant when the donor impurity concentration goes to high for three different geometries. Where $R$ is taken as 1000 Å.

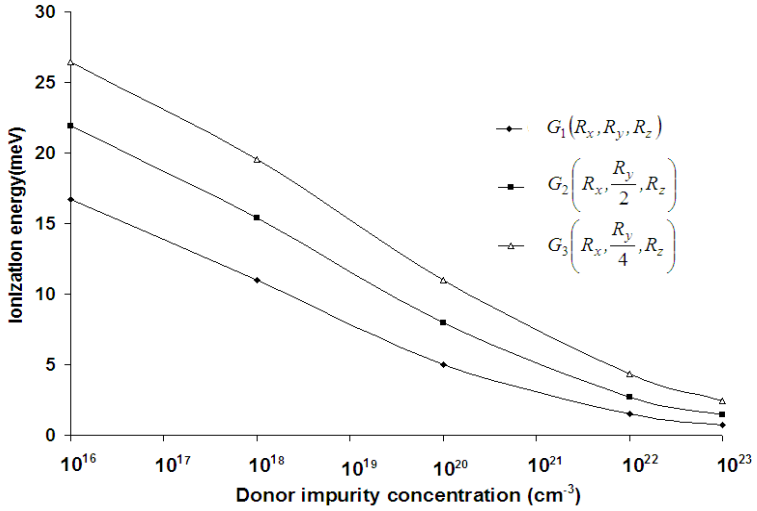



***Fig. 2*** *– Variation of donor ionization energy with concentration for three different geometries*

Fig. 4 exhibits MIT through diamagnetic susceptibility of a donor in a GaAs-$Ga_xAl_{1-x}As$ infinite cubical quantum dot of size $R$ = 1000 Å with the geometry of $G_4(0.5R_x(P), R_y(P), R_z(P))$.. As expected, $\chi_{dia}$ diverges at a critical concentration ($N_c$).This trend is evident from Fig.4. It is observed that MIT takes place at ($N_c$) of $10^{18}$ $cm^{-3}$when pressure and geometry effects are included. At present there are no experimental or theoretical results we couldn't compare our results with the existing literature.

***Table. 1*** *– Variation of effective mass, dielectric constant, and well size of GaAs with pressure*

| **Sr. No** | **Pressure (*Kbar*)** | ***m*(p)* (*a.u*)** | **$\varepsilon$ (*p*) (a.u)** | ***L* (*p*) (*a.u*)** / ***L* (0) = 1000 Å** |
|---|---|---|---|---|
| 1 | 0 | 0.067 | 12.65 | 1887 |
| 2 | 10 | 0.0724 | 11.77 | 1882 |
| 3 | 20 | 0.0783 | 10.89 | 1877 |
| 4 | 30 | 0.0847 | 10.01 | 1872 |
| 5 | 40 | 0.0915 | 9.13 | 1867 |

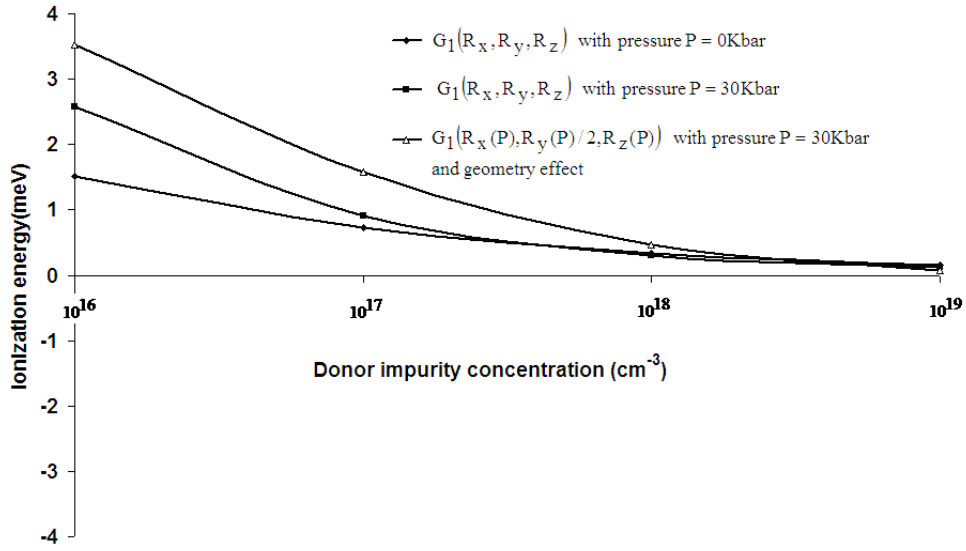
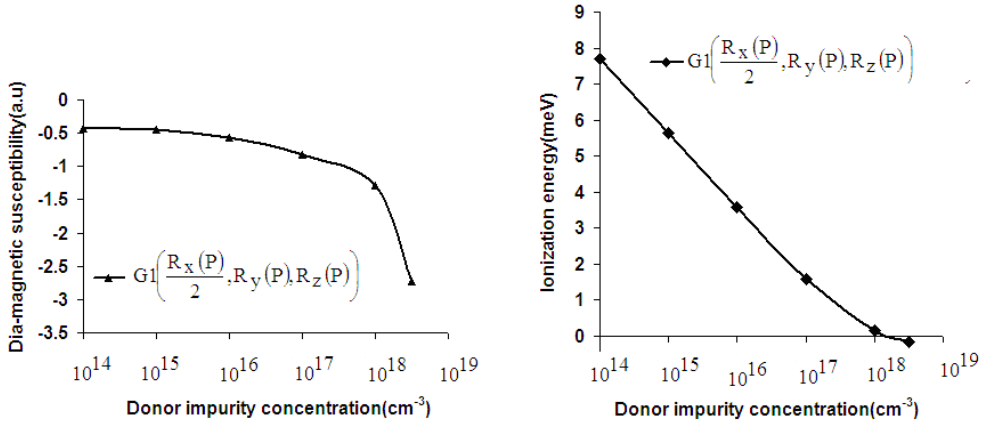



***Fig. 3*** *– Variation of donor ionization energy with concentration for three different conditions*




*a* *b*

***Fig. 4*** *– MIT through diamagnetic susceptibility (a), MIT through ionization energy (b)*

## 4. CONCLUSION

In conclusion of this paper, we have investigated the metal insulator transition in GaAs-$Ga_{1-x}Al_xAs$ cubical quantum dot under simultaneous effects of hydrostatic pressure and geometry by making use of a variational method. It is found that the binding energy increased when the Ly dimension of the system along y axis is reduced by a half and a quarter irrespective of the donor impurity concentrations. In order that, the metal insulator transition couldn't occur quickly at lower concentration of donor impurities in the presence of geometry effect. We believe that our

investigation on simultaneous effects of hydrostatic pressure and geometry on metal-insulator transition in a GaAs cubical quantum dot will stimulate more experimental investigations on these aspects.

One of the authors (S.RS) thanks Prof. K. Navaneethakrishnan (Retd.) and Prof. K. Ramachandaran, School of Physics, Madurai Kamaraj University, Madurai, India, for their useful and valuable suggestions.

## REFERENCES

1. M.J. Kelly, *Low-Dimensional Semiconductors: Materials,Physics Technology, Devices* (Oxford: Clarendon: 1995) and references therein.
2. L. Jacak, P. Hawrylak, A. Wojs, *Quantum Dots*, (Springer-Verlag: Berlin Heidelberg: 1998).
3. J.H. Davies, *The physics of Low-Dimensional Semiconductors, an Introduction*, (Cambridge University Press: 1998).
4. F.J. Ribeiro, A. Latge, *Phys. Rev. B* **50,** 4913 (1994).
5. P.G. Bolcatto, C.R. Proetto, *Phys. Rev. B* **59,** 12487(1999).
6. J. Silva-Valencia, N. Porras-Montenegro, *J. Appl. Phys.* **81,** 901 (1997).
7. H. Schweizer, G. Lehr, F. Prins, G. Mayer, E. Lach, R. Krüger, E. Fröhlich, M.H. Pilkuhn, G.W. Smith, *Superlattices Microstruct.* **12,** 419 (1992).
8. F.J. Ribeiro, A. Latgre, *Phys. Rev. B* **50,** 4913 (1994).
9. H.O. Oyoko, C.A. Duque, N. Porras-Montenegro, *J. Appl. Phys.* **90,** 819 (2001).
10. E. Kasapoglu, H. Sari, I. Sokemen, *Physica E* **19,** 332 (2003)
11. C. Rajamohan, A. Merwyn Jasper D. Reuben, P. Nithiananthi, K. Jayakumar, *J. Math. Chem.* **44,** 743 (2008).
12. H.S. Yang, S. Santra, P.H. Holloway, *J. Nanosci. Nanotech.* **5,** 1364 (2005).
13. Y.A .Yang, O.Chen, A.Angerhofer, Y.C. Cao, *J. Am. Chem. Soc.* **128,** 12428 (2006).
14. S. Rajashabala, K. Navaneethakrishnan, *Physica E* **40,** 843 (2008).
15. M. Latha, S. Rajashabala, K. Navaneethakrishnan, *phys. stat. sol. b* **243,** 1219 (2006).
16. S. Rajashabala, K. Navaneethakrishnan, *Mod. Phy. Lett. B* **20,** 1529 (2006).