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# INVESTIGATION OF THE CONSTANT AND NON-CONSTANT SELF-POLARIZATION UNDER HYDROSTATIC PRESSURE IN AN INFINITE CYLINDRICAL QUANTUM WELL WIRE

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**Abstract**

*This study presents a detailed analysis of the variation in the self-polarization of a cylindrical quantum well wire under external fields with different structure parameters. In the calculations, the variational method and the effective mass approximation are employed, and the calculations are conducted on a GaAs/AlAs infinite cylindrical quantum well wire. In this study, the effects of pressure and magnetic field are considered as external factors, and the variation of self-polarization is examined for different wire radii and impurity positions. Furthermore, for varying wire radii and impurity positions, the self-polarization has been fixed at a specific pressure and magnetic field value. Comparisons have been made for variable pressure and magnetic field values, maintaining this fixed value. It is observed that for certain ranges of hydrostatic pressure variation, the magnetic field must vary more to maintain constant self-polarization. The results obtained are also in line with other studies on self-polarization.*

**Keywords:** hydrostatic pressure, self-polarization

## INTRODUCTION

Due to the confinement of electrons to nanometre dimensions, low-dimensional structures begin to exhibit many quantum mechanical properties such as discrete energy levels. Quantum wells, quantum wires and quantum dots [1-5] are examples of these low-dimensional structures, which can be created using a variety of techniques and have a wide range of applications. With the confinement of charge carriers at small scales, the optical, electronic and magnetic properties of these structures show significant changes due to many factors such as material selection, geometry, temperature, pressure, electric and magnetic fields. By studying these effects and revealing the electronic properties of the material, low power and high-speed devices, quantum computers (qubits), environmentally sensitive sensors, electronic devices and processors can be designed.

Quantum well wires are one of the structures widely used for these purposes. The impurity is one of the important issues in electronic device design. Specifically, in the presence of a impurity atom in quantum wires, the binding energy of the electron to the impurity is calculated using different techniques. One of them, which is widely known, is the variational method [6] and this method is designed to identify the lowest possible energy value for an electron. The binding energy is one of the factors that significantly affect the electronic properties of the structure. Many effects such as temperature, electric field, magnetic field, hydrostatic pressure, laser and different material options are used in the calculations and experimental studies on the binding energy and these factors have a significant effect on the binding energy.

Another topic that has a widespread field of study in quantum wires is polarization. There are many different polarization calculations such as electric field polarization, impurity polarization, self-polarization (SP) [7] in low-dimensional structures. SP is defined as the effect of the




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confinement potential of the structure on the impurity and calculations have been made with many of the above-mentioned parameters for SP in quantum wells, wires and [8] dots.

In this study, the effects of pressure and magnetic field on SP in a cylindrical quantum well wire were investigated for different impurity positions and wire radii. At the end of the study, with a specific choice of pressure and magnetic field, we determine an SP value for each wire radius and impurity position. We investigate the pressure-magnetic field relationship and sensitivity by varying the pressure or magnetic field so that the SP value remained constant. The comparison of the changes in hydrostatic pressure and magnetic field in an infinite cylindrical quantum well wire for a fixed SP have been made for the first time in this study.

## EXPOSITION

The Hamiltonian of a GaAs/AlAs cylindrical wire of radius d in the presence of a magnetic field parallel to the wire axis can be expressed within the effective mass approximation in cylindrical coordinates [9],

$$H = -\frac{1}{2m_e(P)}\left(\vec{P} + \frac{e}{c}\vec{A}\right)^2 - \frac{e^2}{\varepsilon(P)|\vec{r}-\vec{r}_i|} + V(\rho) \quad (1)$$

In this context, the distance between the electron and the impurity atom, represented by $|\vec{r}-\vec{r}_i|$, is given by the expression $(|\vec{\rho}-\vec{\rho}_i|^2 + z^2)^{1/2}$. Here, $\rho_i$ denotes the position of the impurity. The momentum operator is represented by $\vec{P}$, while the vector potential $\vec{A}$ generates a magnetic field in the direction of the wire axis. The effective pressure-dependent mass of the electron is [10],

$$m_e(P) = \frac{m_0}{1+7.51\left[\frac{2}{E_g^\Gamma(P)} + \frac{1}{E_g^\Gamma(P)+0.341}\right]} \quad (2)$$

$m_0$ is the free electron mass and $E_g^\Gamma(P)$ the pressure dependent energy gap for GaAs structure is given by

$$E_g^\Gamma(P) = 1.519 + (1.26x10^{-2})P - (3.77x10^{-5})P^2. \quad (3)$$

$E_g^\Gamma(P)$ and P are expressed in the eV and kbar unit. The pressure-dependent static dielectric constant is as follows: [7,10,11],

$$\varepsilon(P) = (12.74)e^{[-1.73\times10^{-3}P]} \quad . \quad (4)$$

The confinement potential for a cylindrical wire can be expressed as,

$$V(\rho) = \begin{cases} 0, & 0 \le \rho \le d, \\ \infty, & \rho > d. \end{cases} \quad (5)$$

In the absence of hydrostatic pressure, the radius of the cylindrical wire is represented by the value of d. The radii of wire that are dependent on hydrostatic pressure are given by the expression

$$d(P) = d[1 - P(S_{11} + 2S_{12})]. \quad (6)$$

The parameters $S_{11}$ and $S_{12}$ expressed in eq.(6) are $1.16\times10^{-3}kbar^{-1}$ and $3.7\times10^{-4}kbar^{-1}$ [7,11,12].

The Hamiltonian of the system in the cylindrical coordinates in the effective Rydberg unit is expressed as follows, without and with impurity [9],

$$H_{1-2} = -\nabla^2 - \beta\frac{2}{|\vec{r}-\vec{r}_i|} + \gamma L_z + \frac{1}{4}\gamma^2\rho^2 + V(\rho). \quad (7)$$

By setting $\beta$ to zero, the Hamiltonian $H_1$ represents the case in which there is no impurity. Similarly, by setting $\beta$ to one, the Hamiltonian $H_2$ represents the case in which an impurity is taken into account. In this equation, $L_z$ represents the z component of the angular momentum operator, while γ denotes the dimensionless measure of the magnetic field.$(\gamma = e\hbar B/2m_e(T)cR^*)$. The effective Bohr radius and effective Rydberg energy are given by $a^* = \frac{\varepsilon(P)\hbar^2}{m_e(P)e^2}$ and $R^* = \frac{m_e(P)e^4}{2\varepsilon^2(P)\hbar^2}$ respectively.

The electron's ground state wave function without the impurity is given by [13],

$$\psi_1 = N_1 J_0(r_{10}\rho). \quad (8)$$

$J_0(r_{10}\rho)$is an ordinary Bessel Function of order zero $(r_{10} = 2.4048/d)$, The ground state energy of the system without impurity,

$$E_1 = \langle\psi_1|H_1|\psi_1\rangle. \quad (9)$$

The ground state's trial wave function in the presence of an impurity can be selected as, [13],

$$\psi_2 = N_2\psi_1(\rho)e^{(-\lambda|\vec{r}-\vec{r}_i|)}. \quad (10)$$

Here, $N_1$, $N_2$, $\lambda$ and c are the normalization constants, variational parameter and dimensionless impurity parameter respectively and c as follows,

$$c = \rho_i/d. \quad (11)$$

The ground state energy of the system with an impurity is given by the eq.(12) [14-16],

$$E_2 = \langle\psi_2|H_2|\psi_2\rangle_{\lambda_{min}}. \quad (12)$$

SP is defined as the effect of the confining potential of the structure on the impurity and is expressed as [7-9,13],

$$\frac{SP}{e} = -\langle\psi_2|(\rho-\rho_i)\cos\varphi\,|\psi_2\rangle + \langle\psi_3|(\rho-\rho_i)\cos\varphi\,|\psi_3\rangle. \quad (13)$$

In this context, $\psi_3$ represents the wave function of an electron in the absence of a wire potential. It can be expressed as follows: [7-9,13],

$$\psi_3 = N_3 e^{-\frac{|\vec{r}-\vec{r}_i|}{a^*}}. \quad (14)$$

This is the wave function for the ground state hydrogen atom.

In the initial phase of this study, our goal is to clarify the impact of hydrostatic pressure on SP within a cylindrical wire, examining its dependence on magnetic field, wire radius, and impurity position. In the second stage, we determine the SP value for different wire radii and impurity positions under a hydrostatic pressure of 30 kbar, with no magnetic field applied. Subsequently, we gradually decrease the hydrostatic pressure, pinpointing the magnetic field necessary to preserve the SP at its initially determined level. This approach allows us to gain a deeper understanding of the relationship between magnetic field and hydrostatic pressure, when conditions of constant polarization prevail.

In the case where the impurity is taken at the centre of the wire, the electron probability will also be maximum at the centre of the wire. In this configuration (c=0), the potential barriers of the wire remain symmetric with respect to the electron, exerting equal influence from all directions. As a result, SP is negligible, approaching a value close to zero.

Hydrostatic pressure increases the Coulomb interaction between the electron and the impurity by reducing the radius of the cylindrical wire. This results in an increase in the binding energy of the electron. An electron with greater binding energy is less influenced by the wire potential and tends to reduce the SP. Conversely, this situation tends to increase SP when the hydrostatic pressure decreases. Hydrostatic pressure induces substantial variations in the dielectric constant and effective mass of the material. To observe SP, it is essential that the potential barriers create an anti-symmetric effect with respect to the electron. Positioning the impurity at the center maintains the symmetry of the wire barriers with respect to the electron, independent of pressure variations. As a result, the SP remains fixed at zero and is unaffected by changes in pressure. Shifting the impurity away from the wire's center disrupts its symmetry with the wire walls, allowing SP to be measured. In these off-center impurity configurations, increasing hydrostatic pressure subsequently reduces SP, as discussed earlier.

An applied magnetic field adds a symmetric and greater parabolic potential to the system. Therefore, the electron in the wire is trapped with a greater potential and as a result, the impurity-electron interaction increases, the binding energy of the electron increases and greater binding energies tend to reduce SP. It is essential to note that polarization cannot occur if the well walls are symmetric with respect to the electron. Therefore, to observe SP in the presence of a magnetic field, the impurity should be positioned off-center. The magnetic field does not change the dielectric constant and effective mass values of the material, and it does not physically reduce or increase the radius of the wire.

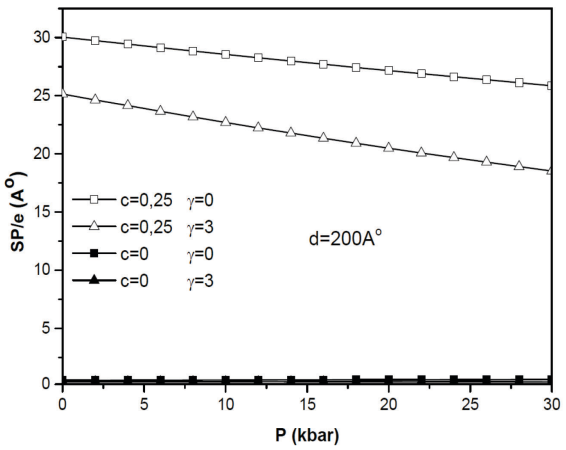


***Fig.1.*** *Variation of the self-polarization with the pressure at a wire radius of 200Å for different magnetic fields and different impurity positions.*

In Fig.1., the hydrostatic pressure varies between 0-30 kbar and the wire radius is selected as 200Å. Two different positions are selected for the impurity atom, the wire center (c=0) and off-center (c=0.25). The change in SP with pressure is plotted by taking the magnetic field zero and $\gamma$ =3 values. From this graphical drawing, it is seen that in the case where the impurity is selected at the center, the symmetry of the wire walls with respect to the electron cannot be disrupted by increasing the magnetic field or pressure, and the SP measurement is not performed. However, for the off-center impurity, the walls are not symmetrical for the electron. The electron is closer to one wall than to the other, which causes it to be more affected by the near wall than by the far wall. An increase in the magnetic field increases the binding energy, leading to a decrease in SP. Similarly, an increase in hydrostatic pressure results in a greater binding energy and a reduction in SP.

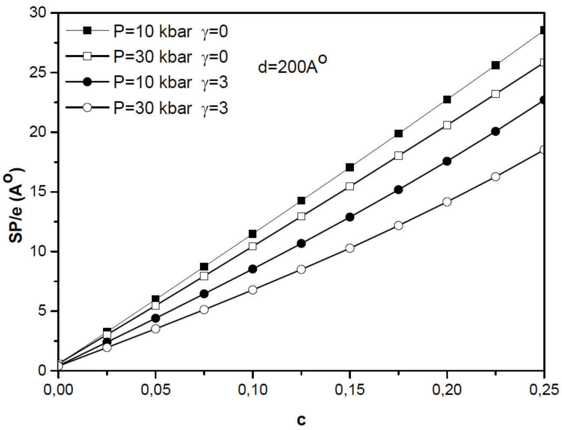


***Fig.2.*** *Self-polarization variation with impurity parameter for different hydrostatic pressure and magnetic field values at 200 Å wire radius.*

The variation of the SP with a dimensionless impurity parameter is shown in Fig.2. In this plot the impurity has been displaced from the centre of the wire to the edge of the wire (c=0 - 0.25) and, the electron is no longer affected by the wire walls to the same extent, hence the symmetry is now broken, and as the impurity moves towards the edge, this anti-symmetric situation for the electron becomes even more pronounced. The electron's wave function cannot move to the edge by the same amount as the impurity because the wire has an infinite potential wall and this causes the electron to position itself so that it remains inside the wire and the wave function is localised inside the wire. While the impurity wants to shift the wave function of the electron with itself, the potential wall it approaches causes this shift to not be the same amount and its distribution to change. The place where the electron has the maximum probability is not same place with the impurity, in other words a shift has occurred and this is the definition of SP. As the impurity moves closer to the edge of the wire, the SP increases. An increase in hydrostatic pressure and magnetic field enhances the binding energy, thereby resulting in a reduction in self-polarization (SP).

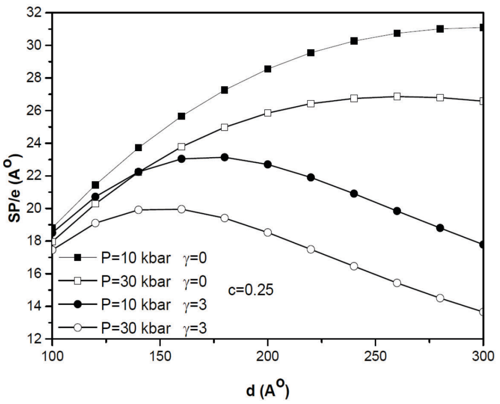


***Fig.3.*** *Self-polarization plots as a function of wire radius for different pressure and magnetic fields with fixed impurity position at c = 0.25.*

In Fig.-3, dimensionless impurity parameter is taken as 0.25 and the wire radius is gradually increased. Since the impurity is far from the center, all SP values remain non-zero and the symmetry of the system is broken at c = 0.25. In small wire radii, the binding energy of the electron is great and the electron is more affected by the wire potential. For small radii, increasing the radius causes a decrease in binding energy and a decrease in the effect of the wire wall on the electron. But in this phase the displacement due to the closeness of the wall to the electron is more effective. However, after a certain wire radius, the effect of the wire potential remains more passive compared to the binding energy and SP decreases or the slope of the increase decreases. In Fig.3., magnetic field and pressure decrease the SP in all cases.

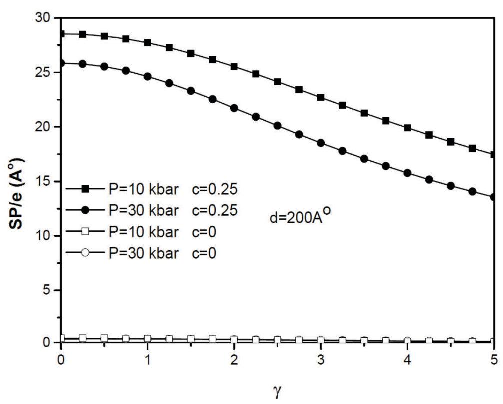


***Fig.4.*** *Effect of magnetic field on self-polarization at d=200 Å for different pressures and impurity positions.*

In support of the above explanations, Fig.4. shows that increasing the magnetic field when the impurity is far from the centre causes a decrease in SP, while no polarization is observed when it is in the centre. For d = 200 Å, hydrostatic pressure reduces SP, while moving the impurity towards the edge of the wire increases SP.

At the final stage of the study, we compared the hydrostatic pressure and magnetic field values with the fixation that gives the same SP value in Fig.5.. We chose $\gamma = 0$ and $P = 30\,kbar$ to fix the SP for each wire radius and impurity positions [$SP = 20.59$Å for $d = 200$Å $and\ c = 0.2$; $SP = 42.77$Å for $d = 200$Å $and\ c = 0.4$; $SP = 14.29$Å for $d = 100$Å $and\ c = 0.2$; $SP = 29.63$Å for $d = 100$Å $and\ c = 0.4$ ]. We have seen that the $\gamma$-P variations that ensure that the SP remains constant are linear, but after the pressure value of 25 kbar, it requires greater reductions in the magnetic field.

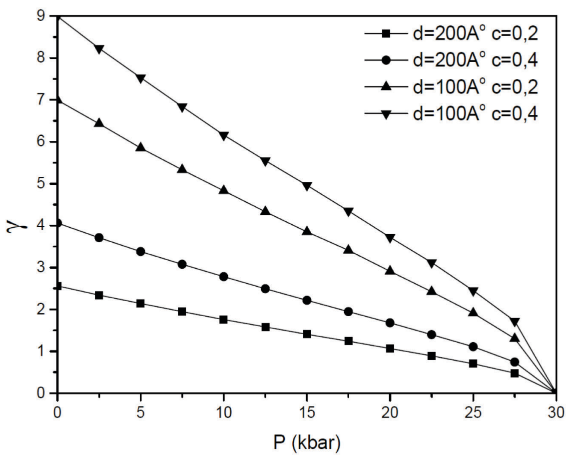


***Fig.5.*** *Hydrostatic pressure-magnetic field variation for a fixed self-polarization (at* $\gamma = 0$ and $P = 30\,kbar$ *) for different wire radii and impurity positions.*

Again from this graph we can see that the magnetic field values that will tolerate the change in SP that will occur with the change in pressure in wires of smaller radius show a significant increase and that a greater magnetic field change is required to neutralize the change in SP with pressure in cases where the impurity approaches the edge.

## CONCLUSION

In conclusion, it has been shown that SP decreases with increasing hydrostatic pressure in an infinite cylindrical GaAs/AlAs quantum wire. However, some effects, such as the magnetic field values, can be adjusted to ensure that the SP remains constant under pressure changes. Thus, by performing a dual investigation of the effects that change the SP, it can be determined which effect causes more effective changes in SP or causes greater changes. In the light of the data obtained, it can be seen that the magnetic field should change more to keep SP constant for values of pressure greater than 25 kbar. Furthermore, a crucial conclusion from this analysis is that the effect of the parameters on SP should not be interpreted in isolation. Instead, the interplay of multiple parameters must be evaluated to gain a comprehensive understanding. It is also important to note that certain values in the graphs may overlap, indicating that similar outcomes can be produced by varying combinations of parameter values. This nuance should be carefully considered when interpreting the results.

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