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Orbital Quantum Bit in Si Quantum Dots

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Abstract

In this paper, current status of experimental and theoretical work on quantum bits based on the semiconductor quantum dots in the University of Seoul will be presented. A new proposal utilizing the multi-valley quantum state transitions in a Si quantum dot as a possible candidate for a quantum bit with a long decoherence time will be also given. Qubits are the multi-valley symmetric and anti-symmetric orbitals. Evolution of these orbitals is controlled by an external electric field, which turns on and off the inter-valley interactions. Initialization is achieved by turning on the inter-valley Hamiltonian to let the system settle down to the symmetric orbital state. Estimates of the decoherence time is made for the longitudinal acoustic phonon process.

Keywords : Si Quantum dots, Obital quantum bits, Inter-valley interactions

I. Introduction

It is well known that the lowest conduction band of an ideal Si crystal has six equivalent minima of ellipsoidal shape along the [100] direction as shown in figure 1. These ellipsoids are often called as valleys and the total wave function of the ground state is obtained from a linear combination of the six wave functions each localized around one of the Δ_1 conduction-band minima. The overlap of wave functions associated with different valleys is assumed to be negligible.

In the study of early quantum structures such as n-channel inversion layer on the Si (001) surface, it was found that the broken translation symmetry lifts the six-fold degeneracy into the two-fold degenerate valleys located near the X point in the <001> direction in the k-space and the four-fold degenerate valleys in the direction normal to the surface [1].

In addition, there were experimental observations [2-4] of anomalous structures in the gate-voltage dependence of the conductivity of vicinal planes of Si (100) n-channel inversion layers. It has been suggested that these anomalous structures are caused

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by the lifting of two-fold valley degeneracy in the <001> direction as a result of valley-valley interaction [5,6]. The splitting is turned out to be proportional to the gradient of the confinement potential normal to the surface [7].

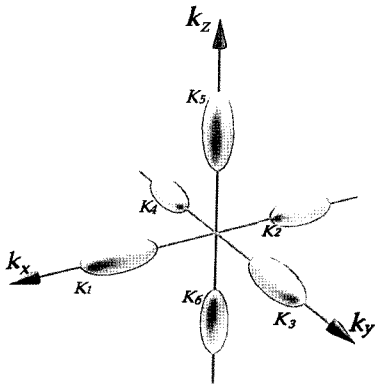


Fig. 1. The lowest conduction band of an ideal Si crystal with six equivalent minima of ellipsoidal shape along the [100] direction.

It would be an interesting query to ask whether the inter-valley coupling is controllable. If that were possible, it would permit us more degrees of freedom in silicon technology. It could also lead to the potential applications to the silicon based quantum information processing. So far, most of the existing proposals for the solid state quantum bits (qubits) are based on the electron spin confined in the quantum-dots [8,9], coherent quantum state in a Cooper-pair box [10], or the nuclear spins of impurity atoms implanted on the surface of Si [11,12]. For the latter it still remains an experimental challenge to fabricate a structure in which each nuclei can be effectively manipulated. Recently, there have been observations of coherent oscillation of a charge qubit in a III-V double quantum dot [13] and stacked coupled quantum dot structures [14]. These results suggest that the controlled evolution of superposed charge states could be possible in the semiconductor quantum dots. In order to implement the solid state quantum computation, however, it is required to minimize the decoherence effects on the coherent quantum states or qubits [15]. Potential drawbacks of these compound semiconductor charge qubits are relatively short decoherence time and difficulties in fabricating double dots. There would be several merits of a silicon implementation of quantum bits if it is possible. First of all, the crystal growing and processing technology for Si is quite matured. Secondly, some of the scattering processes which contribute to the decoherence such as intra-valley optical phonon processes are forbidden inherently from the group theoretical considerations in the case of silicon and within each ellipsoid (intra-valley) is limited to acoustic phonons and impurities [16].

II. Theoretical Model

Let's consider the quantum dot of cube geometry with the z-direction assumed to be along the Si (001) surface. Based on Kohn-Luttinger effective mass theory [17], the envelope function for the quantum states in a Si quantum dot is given by

$$F(\vec{r}) = \sum_{\vec{k}} F(\vec{k}) \exp(i\vec{k} \cdot \vec{r}) \tag{1}$$

and

$$F(\vec{k}) = \sum_{i} \alpha_i F_i(\vec{k}) \tag{2}$$

where $F_i(\vec{k})$ is centered about the ith minimum. The constants α_i can be determined from the group theoretical considerations [18-20]. The equation of motion for $F_i(\vec{k})$ becomes

$$\varepsilon_i(\vec{k}) F_i(\vec{k}) + \sum_{j} \sum_{\vec{k}'} D^{ij}_{\vec{k},\vec{k}'} V(\vec{k} - \vec{k}') F_j(\vec{k}') = \varepsilon F_i(\vec{k}) \tag{3}$$

where $\varepsilon_i(\vec{k})$ is the energy dispersion relation of the i-th valley, $V(\vec{k})$ the Fourier component of the total potential, and $D^{ij}_{kk'}$ is the inter-valley coupling term which can be derived from the cell periodic

function for the conduction band.

Then within the frame of multi-valley effective mass theory [21,22], the equation of motion for $F_l(\vec{r}) = \sum_{\vec{k}} F_l(\vec{k}) \exp(i\vec{k} \cdot \vec{r})$ can be written down as

$$\left[H_l(-i\vec{\nabla}) + V(\vec{r}) - E\right]F_l(\vec{r}) + \sum_{l' \neq l} H_{ll'}(\vec{r}, -i\vec{\nabla})F_{l'}(\vec{r}) = 0 \tag{4}$$

Here,

$$H_l(-i\vec{\nabla}) = -\frac{\hbar^2}{2m_x}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_y}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2} - \frac{ie\hbar B}{2m_x} y\frac{\partial}{\partial x} - \frac{ie\hbar B}{2m_y} x\frac{\partial}{\partial y} + \frac{e^2B^2}{8}\left(\frac{x^2}{m_y} + \frac{y^2}{m_x}\right) \tag{5}$$

and

$$\begin{aligned} & H_{ll'}(\vec{r}, -i\vec{\nabla}) \\ & = I_{ll'} \exp[-i(\vec{K}_l - \vec{K}_{l'}) \cdot \vec{r}](V(\vec{r})) \\ & -i(\vec{J}_{ll'} \cdot \vec{\nabla})\exp[-i(\vec{K}_l - \vec{K}_{l'}) \cdot \vec{r}](V(\vec{r})) \\ & + \exp[-i(\vec{K}_l - \vec{K}_{l'}) \cdot \vec{r}](V(\vec{r}))(-i\vec{J}'_{ll'} \cdot \vec{\nabla}) \end{aligned} \tag{6}$$

and

$$V(\vec{r}) = V_c(\vec{r}) + e\vec{F} \cdot \vec{r} \tag{7}$$

where m_x, m_y, m_z are effective masses along x, y, z directions in each valley, E is quantized energy, $\vec{K}_l$ is the wave vector at the minimum at the l-th valley, $I_{ll'}, \vec{J}_{ll'}, \vec{J}'_{ll'}$ are inter-valley coupling terms, $V_c(\vec{r})$ is the quantum dot confinement potential, and $\vec{F}$ is an applied electric field.

III. Numerical Results and Discussions

We have solved equations (4) to (7) for the Si quantum dot structure mentioned above numerically and considered potential quantum bit operation utilizing the inter-valley interactions. Quantum dot potential is assumed to be infinite at the boundary and zero inside the dot in the absence of an applied electric field. In this work we considered a quantum dot with the dimension of 8 nm, 12 nm, and 6 nm in x-, y- and z-directions, respectively. In this structure, the ground state is associated with doubly degenerate valleys 5 and 6. When the weak static magnetic field is applied along the growth direction, the ground state wave function is composed of the linear combination of p-like T_1 states [24], the irreducible representations of T_d symmetry of the Si crystal. These orbitals satisfy the following effective Hamiltonian in the interaction picture:

$$H = \begin{bmatrix} \varepsilon(F) & \Delta(F) \\ \Delta(F) & \varepsilon(F) \end{bmatrix} \tag{8}$$

Here ε is the energy difference between symmetric and anti-symmetric states, Δ is the inter-valley coupling, and F is an external electric field along the z-direction. When $F = 0$, both ε and Δ are zero and the total state remains as it was because there is no inter-valley coupling. In this simple model we have neglected the coupling of orbitals between different axes. For example, the coupling between valleys 1 and 5 (x-axis and z-axis) is found to be a million times smaller than the coupling between the valleys 5 and 6 (both are in z-axis). If we apply an external electric field to the quantum dot, the inter-valley interaction is turned on and doubly degenerate ground state is splitted. The crystal momentum necessary for the electron states between the valley 5 and the valley 6 to be coupled is provided by an applied electric field along the z-direction [16].

In Fig. 2, we plot the energy difference ε between the symmetric and the anti-symmetric states as well as the inter-valley coupling energy Δ which is defined as $\Delta(F) = \langle F_5 | H_{56} | F_6 \rangle$. In this figure, one can see that the inter-valley coupling is increasing rapidly with the electric field. For example, the calculated values of ε and Δ are 63.5 μeV and 31.6 μeV, respectively, when F=400 kV/cm. When F is increased to 500 kV/cm, we

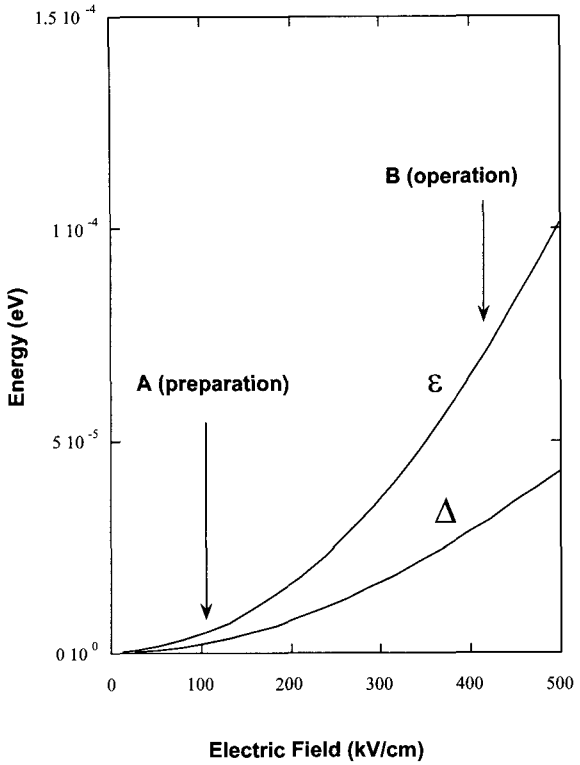


Fig. 2. We plot the energy difference ε between the symmetric and the anti-symmetric states as well as the inter-valley coupling energy Δ of a Si quantum dot as functions of the electric field.

have $\Delta = 43\,\mu eV$.

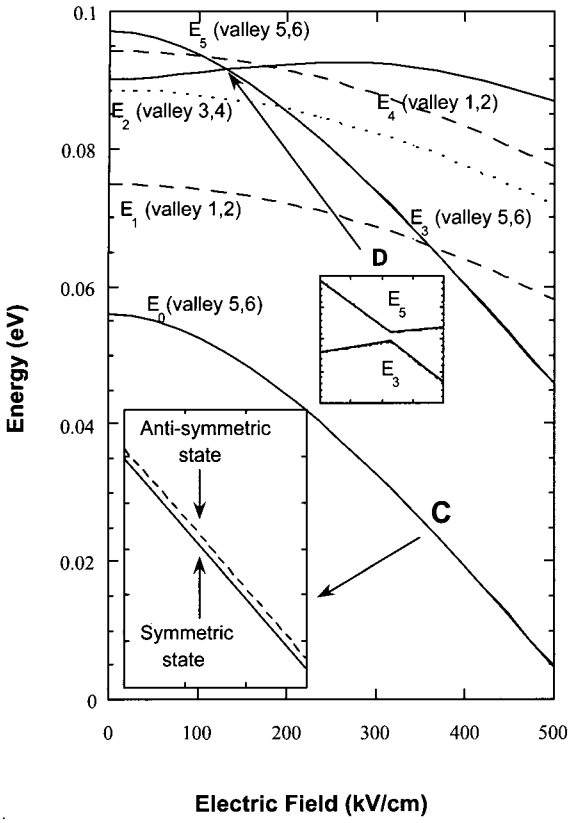
If we turn on the electric field and wait long enough, then the system will be in the symmetric state which will be denoted as |0>. The coherent evolution from the symmetric state |0> to the anti-symmetric state |1> could be observed by applying the sharp voltage pulse to the pulse gate as has been done for the Cooper-pair box [10] or the double quantum dot structure [13,14].

The coherent oscillation of the system is expected with the angular frequency given by $\Omega = \sqrt{\varepsilon^2 + \Delta^2}/\hbar$, which corresponds to the microwave frequency of 17.2 GHz. When the system is evolved to the state |1> and if we turn off the electric field F adiabatically, then the inter-valley coupling is turned off and the resulting state would be the anti-symmetric orbitals which would maintain its phase coherence until the decoherence destroys it.

Figure 3 shows the first 6 energy levels associated with valley 5 (or 6) in solid lines, valley 1 (or 2) in dashed lines, and valley 3 (or 4) in dotted line as functions of increasing electric field. Weak magnetic field of 1.5 Tesla is applied along the z-axis. The dimension of the quantum dot used in this particular calculation is such that the ground state is associated with valley 5 or 6 in the absence of an external field. It is interesting to note that the slopes for the valleys 1 and 3 are similar but they are different from those of the valley 5 because of the effective mass difference along the field direction. The energy states are labeled for the single valley case, that is, when the intervalley coupling is ignored. Part of the ground state energy level is magnified and shown in the small box inside the figure 3. One can notice that the ground state energy is further splitted into symmetric and anti-symmetric states. It is interesting to see that E_3 and E_5 associated with valleys 5 and 6 show anti-crossing at point D with increasing electric field. The inset shows the magnification of point D.

At low electric field, E_3 is pushed up while E_5 is showing the negative shift with increasing electric field until anti-crossing point D and their behaviors are changed the other way around after passing D. Similar behavior was observed in the case of quantum well with applied electric field [25]. The insets of Fig. 3 shows a magnified energy diagrams. We first consider the symmetric and anti-symmetric states associated with E_0 (point C). Initially, we set the electric field at a low value (point A) so that the transition between two states is difficult to occur (Fig 2) due to a relatively small transistion probability. The electron in the quantum dot is in the ground state When the gate bias is switched to a higher electric field (point B), the time evolution between two states begins.

The time interval of the pulse determines the relative population of two states and they remain at the final values when the pulse is switched back to A. The rise time of the pulse should be shorter than $\hbar/\Delta$ at A and longer than $\hbar/\Delta$ at B.



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