SUMMARY OF Ph.D. DISSERTATION

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Title

Theoretical study of electronic states in silicon quantum dots

Abstract

The electronic and spin states in silicon (Si) single quantum dots and double quantum dots are theoretically examined taking account of multivalley structure in conduction band.

For Si single quantum dots, we calculate the one-electron levels using effective mass approximation, in the case of two equivalent valleys. The ground state is determined by evaluating the Coulomb and exchange interactions numerically. In magnetic fields, Zeeman effect is considered. We find that the multivalley structure results in the degenerate one-electron levels of different valleys. Owing to no spin coupling between these levels, different spin states are degenerate in energy. When the dot size is less than 10 nm, electrons occupy the lowest levels in different valleys in the absence of spin coupling. Highest spin states are realized by applying a small magnetic field. This is different from the case of GaAs quantum dots, where high spins appear due to the exchange interaction in exceptional cases with orbital degeneracy (Hund's rule). When the dot size is much larger, electrons are accommodated in a valley, making the highest spins, to gain the exchange energy. In the presence of intervalley scattering due to impurities, sharp edges of the confinement potential etc., low-spin states often appear, reflecting the splitting of degenerate levels.

In Si double quantum dots, the exchange couplings between localized spins are examined, considering two degenerate one-electron levels in a quantum dot. There are two kinds of tunnel couplings between two quantum dots, intravalley and intervalley tunnel couplings. We determine the ground and excited states taking accounts of intradot and interdot Coulomb interaction exactly. The exchange couplings do not work without intervalley tunneling nor intervalley scattering in a quantum dot, whereas they work with intervalley tunneling. We estimate the magnitude of the exchange couplings and discuss the problems to apply the quantum dots to quantum information processing.

Finally, the one-electron levels are examined using the tight-binding model to consider the atomic structure of Si quantum dots. To examine the valley degeneracy, the energy difference between the lowest two levels by the confinement potential is investigated. For the confinement potential, we study two situations, one is for the quantum dots formed by gate electrode and the other is for those fabricated by oxidation. We find that the energy splitting is not large except in extremely small quantum dots and justify the calculations using effective mass approximation.