Energy Levels of an Off-centered Impurity in Si/SiGe/Si Quantum Dots

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Terahertz radiation from δ-doped SiGe/Si quantum well (SGQW) has been observed in the near recent [1]. The mechanism of the radiation was proposed to be dominated by the impurity levels that are separately attached to light-hole and heavy-hole bands [1,2]. It is particularly true in quantum dot (QD) structure due to the carrier restricted to move in a quasi-zero-dimensional geometry.

A theoretical model for an off-centered impurity in Si/SiGe/Si quantum dot (QD) under high electric field (directed to z-axis) is presented. In this model, the QD assumes to be defined approximately by a parabolic confinement potential, and the impurity permits to be deviated away from the center of the dot along the field direction. The variational method is applied to estimate the energy levels of 0s, 0p₀ and 0p± states.

We apply our theory to the system of doped-SiGe/Si QD. The material parameters of SiGe are obtained by linearly interpolating approach for the Ge mole fraction x = 0.5. The parameters we found are given as: the valence-band offset 299meV, heavy-hole mass 0.385m₀, dielectric constant 13.93ε₀, effective Bohr radius 19.174 angstroms, and the effective Rydberg 26.9175meV. Fig.1 shows the dispersions of 0s, 0p₀, and 0p± states with respect to the field strength for the dot size L₀ = 1.456nm and z₀ = 0, where E₁ and E₂ are the lowest and the second lowest subbands of the dot, respectively. The field strength Vᵣ = 1Ry can be converted to the real electric-field strength F = 140385V / cm. The 0p₀ state appears to be more dispersive than 0s and 0p± states, since the 0p₀ state has a greater change in momentum along the field direction than others states. From the figure, one finds the 0p₀ state approaches the 0s state for a large electric field. This feature also appears in the plots, in Fig.2, of the transition energies between 0p₀ and 0s states and between 0p± and 0s states with respect to the field strength.

References:

Fig.1. Dispersions of 0s, 0p₀, and 0p± states (solid line), and the dispersions of the lowest and the second lowest subbands (dashed line), with respect to the electric-field strength for L₀ = 1.456nm.

Fig.2. Transition energies between 0s and 0p₀ states and between 0s and 0p± states as a function of the field strength with L₀ = 1.456nm and z₀ = 0.