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Crystal orientation effect on intersubband transition properties of (11n)-oriented ZnCdTe/ZnTe semiconductor quantum dots

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ABSTRACT

Crystal orientation effects on intersubband transition properties of (11n)-oriented ZnCdTe/ZnTe quantum dots (QDs) were investigated by using the continuum elasticity and effective mass theories. In a range of the crystal angle below 30°, the subband energy difference is nearly independent of the crystal angle. On the other hand, it gradually increases with crystal angle θ when the angle exceeds 30° and becomes a maximum near the angle ($\theta = 55°$) corresponding to a (111) crystal orientation due to the piezoelectric field effect. The transition matrix element becomes a maximum near the angle $\theta = 15°$ and a minimum near the crystal angle $\theta = 60°$.

1. Introduction

Much attention is presently being paid to the physics of low-dimensional semiconductor structures, among which quantum dots (QDs) are of particular interest because their electronic and optical properties dramatically change as the size of the QD varies [1,2]. Currently, III–V materials are the leading ones for the fabrication of QDs. On the other hand, recently, the II–VI materials have attracted increasing attention due to their large band gap and their potential applications in short-wavelength optoelectronic devices [3–5]. Among them, the ZnCdTe/ZnTe material system is interesting from the point of fabrication of QDs since the lattice mismatch between these two constituents is similar to that of GaInAs/GaAs system, which is the most widely studied system in the context of QDs. Advances in a growth technology of II–VI semiconductors now permit the growing of high-quality ZnCdTe/ZnTe QDs [6,7]. With the current process in the crystal growth, it will be interesting to investigate crystal orientation effects on optical properties of semiconductor QD structures because the crystal orientation will significantly modify the strain-induced band structures. The (001)-oriented zinc-blende structure semiconductors do not have strain-induced polarization fields. However, it has been reported that strained quantum well (QW) structures with any other growth direction have the internal field due to piezoelectric polarizations [8]. Thus, the detailed knowledge of the internal potential and the strain field in and around the QDs can serve as a useful tool to understand their electronic and optical properties. On the other hand, despite its importance, related theoretical investigations of crystal orientation effects on their optical properties are scarce in the literature.

In this research, we investigate crystal orientation effects on intersubband transition properties in the conduction band of (11n)-oriented ZnCdTe/ZnTe semiconductor QDs by using the continuum elasticity and the effective mass theories. The pyramidal ZnCdTe QD is assumed to be located at the center of a ZnTe matrix of a cuboidal shape having a volume of $2a \times 2b \times 2c$ centered at the origin ($a = b = c = 100$ Å). The Hamiltonian is solved by using a three-dimensional finite-element method (FEM) formulation [9–11].

2. Theoretical model

Off-diagonal strains in zinc-blende structure semiconductors induce a polarization given by [8]

$$P_i^S = 2e_{14}\epsilon_{jk}, \tag{2.1}$$

where P^S is the induced polarization, e_{14} is the piezoelectric constant, and $i,j,k = x,y,z$. Here, i,j,k are in cyclic order. A strained layer with a [001] growth direction has only diagonal strains. Thus, the (001)-oriented layer will not have strain-induced piezoelectric polarization fields. However, strained layers with any other growth direction have piezoelectric polarization fields. In the case of the QW structure, the piezoelectric polarization along the growth

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direction is important because the electric field in the QW originates from polarization charges at heterojunction interfaces. On the other hand, in the case of QD structure, piezoelectric polarizations along all directions are important because QDs yield surfaces along x, y, z directions.

We need to know ϵ_{yz}, ϵ_{xz}, and ϵ_{xy} to obtain $P_x{}^S$, $P_y{}^S$, and $P_z{}^S$. The biaxial strain components ϵ_{yz}, ϵ_{xz}, and ϵ_{xy} for the (11n)-oriented zinc-blende crystal are given by

$$\epsilon_{yz} = \frac{n(\epsilon'_{zz}-\epsilon'_{xx})}{n^2+2} + \frac{\epsilon'_{xz}(n^2-2)}{\sqrt{2}(n^2+2)},$$
$$\epsilon_{xz} = \epsilon_{yz},$$
$$\epsilon_{xy} = \frac{(\epsilon'_{zz}-\epsilon'_{xx})}{n^2+2} + \frac{\sqrt{2}\epsilon'_{xz}n}{n^2+2}. \quad (2.2)$$

Also, the biaxial strain components ϵ'_{ij} in the primed coordinate for the (11n)-oriented zinc-blende crystal are given by

$$\epsilon'_{xx} = \epsilon'_{yy} = \epsilon_{\parallel},$$
$$\epsilon'_{xy} = \epsilon'_{yz} = 0,$$
$$\epsilon'_{zz} = -2\frac{K_3}{\sqrt{2}K_2}\epsilon_{\parallel},$$
$$\epsilon'_{xz} = -2\frac{K_1}{\sqrt{2}K_2}\epsilon_{\parallel}, \quad (2.3)$$

where

$$K_1 = (C_{11}+2C_{12})(-C_{11}+C_{12}+2C_{44})n(n^2-1),$$

$$K_2 = 2C_{11}C_{44}+2C_{12}C_{44}+4C_{44}^2+(C_{11}^2+C_{11}C_{12}-2C_{12}^2 +2C_{11}C_{44}-4C_{12}C_{44}+C_{11}C_{44}n^2)n^2,$$

$$K_3 = -2[C_{11}C_{44}+3C_{12}C_{44}-2C_{44}^2+(C_{11}^2+C_{11}C_{12}-2C_{12}^2 -C_{11}C_{44}+C_{12}C_{44}n^2)n^2], \quad (2.4)$$

and C_{ij} are the stiffness constants in the strained epilayers. Here, $\epsilon_{\parallel} = (a_s-a_e)/a_e$, and a_s and a_e are lattice constants for the substrate and epilayer materials, respectively. Then, the polarizations in the (x', y', z') coordinates are given by

$$P_{x'} = \frac{(\cos\theta\cos\phi P_x^S + \cos\theta\sin\phi P_y^S - \sin\theta P_z^S)}{\sqrt{(\cos\theta\cos\phi)^2+(\cos\theta\sin\phi)^2+(\sin\theta)^2}}$$

$$P_{y'} = \frac{(-\cos\theta\sin\phi P_x^S + \cos\theta\cos\phi P_y^S - \sin\theta P_z^S)}{\sqrt{(-\cos\theta\sin\phi)^2+(\cos\theta\sin\phi)^2+(\sin\theta)^2}}$$

$$P_{z'} = \frac{(\sin\theta\cos\phi P_x^S + \sin\theta\sin\phi P_y^S + \cos\theta P_z^S)}{\sqrt{(\sin\theta\cos\phi)^2+(\sin\theta\sin\phi)^2+(\cos\theta)^2}}, \quad (2.5)$$

where $\cos\theta = n/\sqrt{2+n^2}$ and $\cos\phi = 1/\sqrt{2}$ for the (1 1 n)-oriented crystal. The vectors of the stress σ and the electric flux D are related to the strain ϵ and electric field E vectors as [12]

$$\sigma_{ij} = C_{ijlm}\epsilon_{ij} - e_{kji}E_k,$$
$$D_i = e_{ijk}\epsilon_{jk} + \epsilon_0\epsilon_r E_j, \quad (2.6)$$

where C_{ijlm}, e_{kji}, and ϵ_r are the elastic moduli, piezoelectric coefficients, and relative dielectric constants, respectively. The elastic strain and piezoelectric potential were calculated using the theory of continuum elasticity and FEM [10,11]. The effective-mass Hamiltonian H_0 is given by

$$H_0 = -\frac{\hbar^2}{2m_c}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + a_c(\epsilon_{xx}+\epsilon_{yy}+\epsilon_{zz}) +E_c(x,y,z)+|e|V_p(x,y,z), \quad (2.7)$$

where a_c is the deformation potential for the conduction band, E_c is the energy of conduction-band edge without strain and piezoelectric field, and V_p is the piezoelectric potential.

3. Results and discussion

Fig. 1 shows (a) piezoelectric polarization and (b) strain as a function of the polar angle θ with the azimuthal angle ϕ fixed at $\pi/4$ for strained pyramidal $Zn_{0.1}Cd_{0.9}Te/ZnTe$ QD structure. The base of the pyramidal QD is assumed to be located at the center of a ZnTe matrix with a cuboidal shape having a volume of $2a \times 2b \times 2c$ centered at the origin ($a = b = c = 100$ Å). The wetting layer thickness is set to be 20 Å while that of the capping layer is set to be 100 Å. The pyramidal QD is parameterized by the length of the base, a, and the height, h. Here, we set $h = a/2$. The length of the base and the height for QD are set to be $a = 100$. We know that polarizations along x', y', and z' are zero at $\theta = 0$, which corresponds to a (001) crystal orientation. That is, a strained layer with a [001] growth direction has only diagonal strains and does not

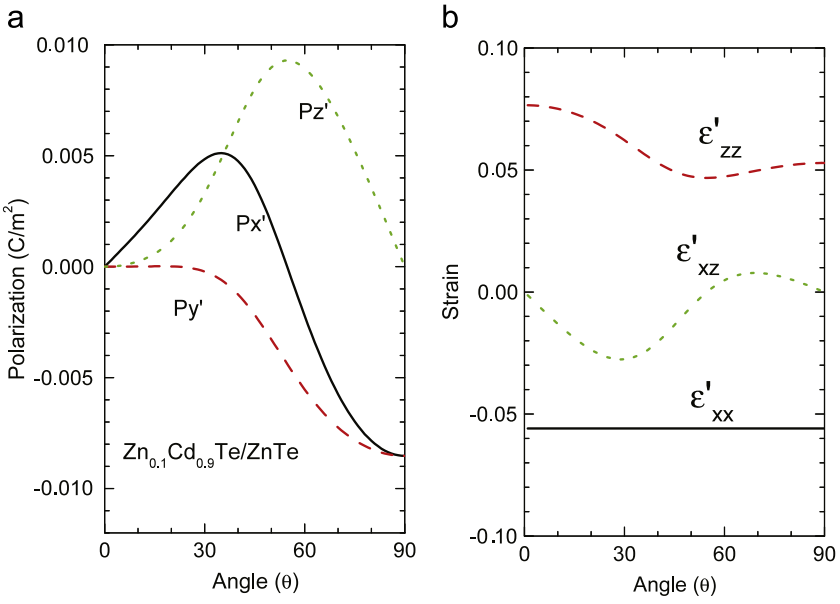

Fig. 1. (a) Piezoelectric polarization and (b) stain as a function of the polar angle θ with the azimuthal angle ϕ fixed at $\pi/4$ for strained pyramidal $Zn_{0.1}Cd_{0.9}Te/ZnTe$ QD structure.