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Electronic States in Semiconductor Quantum Dot with Fluctuating Interfaces

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Effects of interface fluctuations on the electronic states in semiconductor quantum dots are analyzed on the basis of numerical solutions for ground state wave functions and energy eigenvalues. It is shown that the effective volume of confinement becomes smaller than the real volume of quantum dots due to fluctuation. This effect comes from the fact that the wave functions with larger characteristic wavelength are not able to deform themselves following the fluctuation of interfaces exactly.

1. INTRODUCTION

Recent progresses in semiconductor technologies have made it possible to fabricate semiconductor microstructures, such as quantum wires or wells whose dimensions are less than 100 nm. In the fabrication process of such microstructures, it is very difficult to have geometrically well-defined interfaces of heterojunctions on the atomic scale and fluctuations of interfaces of the order of several atomic layers are usually inevitable[1–3]. These fluctuations may influence electronic states in microstructures and also characteristics of devices composed of these microstructures. The purpose of this paper is to analyze the effect of such fluctuations on the ground state energy of electrons confined in quantum dots or wells.

We have been developing the computational codes based on the density-functional theory and the finite element method in order to analyze the electronic states in various semiconductor microstructures[4, 5]. In this paper, we apply our codes to the cubical quantum dots with interface fluctuations and compute the shifts of eigenvalues of the ground state due to fluctuations. We expect that the effects of interactions between electrons on the shifts of the eigenvalues may be small and neglect electronic many-body effects.

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The cross section of our quantum dot is shown in Fig.1. Electrons are confined by the conduction band offset between GaAs (well) and $Al_xGa_{1-x}As$ (barrier). The average dimension of the well part is $\frac{7}{8}L \times L \times L$ with fluctuations in the positions of interfaces. In what follows, we take the size of well part as $L = 100$Å and the thickness of barrier part as $L' = 67.5$Å. We analyze mainly the case where parallel two interfaces fluctuate with some periods.

The effective mass approximation and the finite element method are used to solve the Schrödinger equation. As the boundary condition, we assume that the wave function is zero at outer boundary of $Al_xGa_{1-x}As$. The validity of the boundary condition will be discussed in the next section.

We determine the ground state eigenvalues corresponding to various fluctuating interfaces in both cases where the values of the conduction band offset are 0.2eV and 60eV and discuss the effective volume in which electrons are confined.

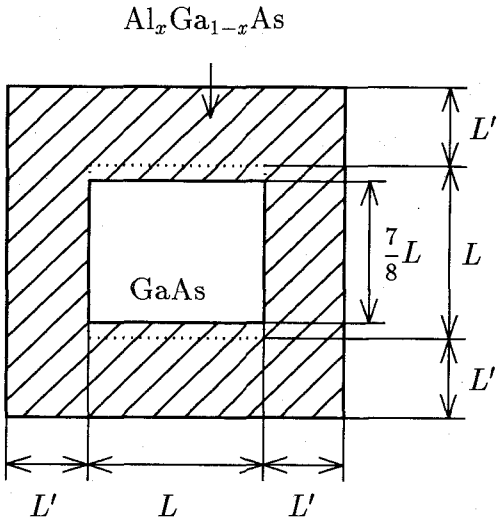

Fig.1. Cross section of quantum dot.

2. FORMULATION

We adopt the effective mass approximation with the effective mass $m^* = 0.067m_e$, assuming electrons are in the conduction band of GaAs. We expect that the effects beyond the effective mass approximation may have small influence on the shift of eigenvalues due to fluctuation.

The eigenvalues and wave functions in our system are determined by the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 + v(\mathbf{r})\right)\psi_i(\mathbf{r}) = E_i\psi_i(\mathbf{r}), \tag{1}$$

where $v(\mathbf{r})$ is an external potential. The external potential $v(\mathbf{r})$ consists of two parts. One is the part surrounding the $L \times L \times L$ quantum dot and another is the potential due to fluctuating interfaces. The interface fluctuations are assumed to occur mainly on two faces of

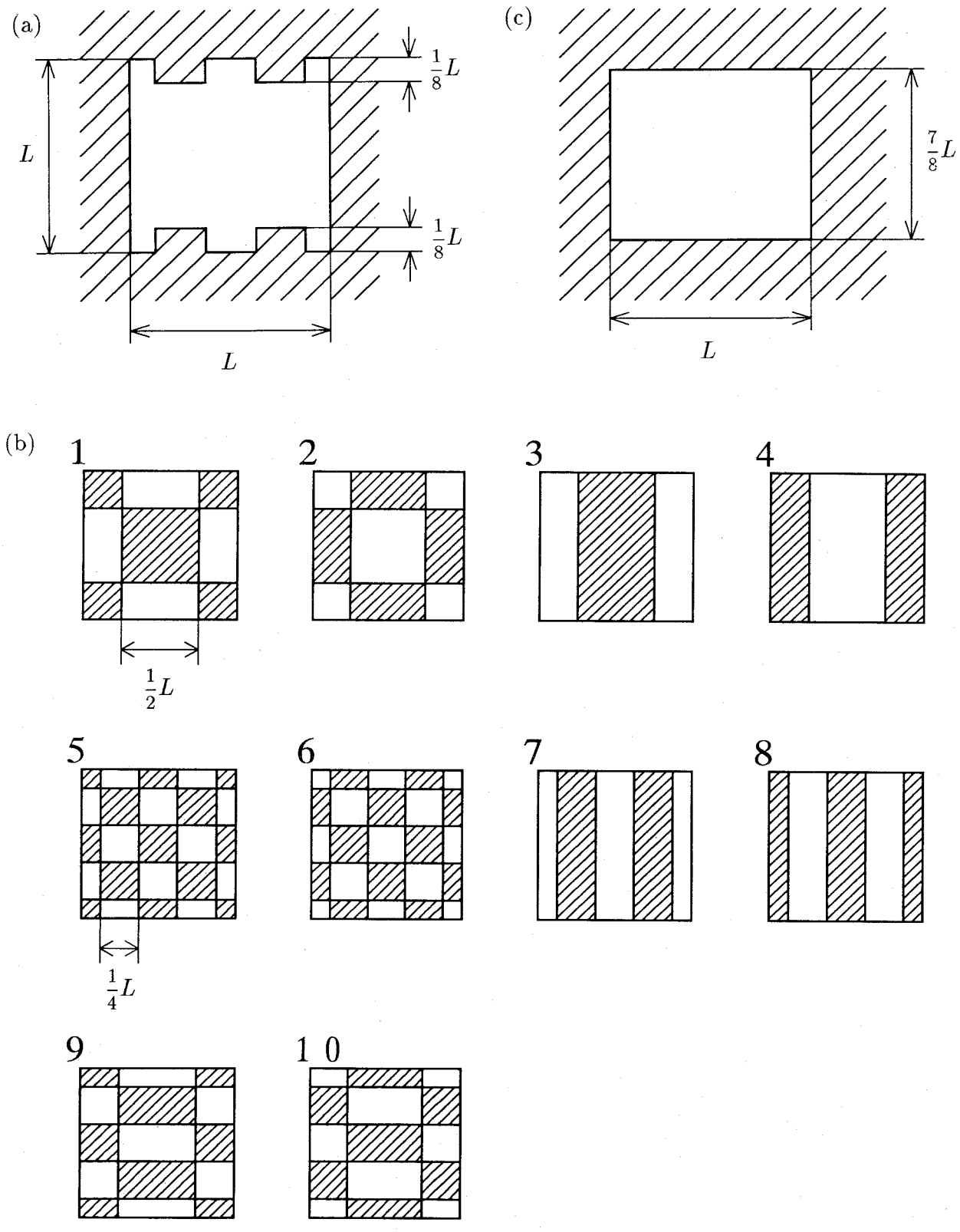

Fig.2. (a)Example of cross section of quantum dot with fluctuating interface. (b)Patterns of fluctuating interfaces. (c)Cross section of quantum dot without fluctuation to which all cases reduce when fluctuations are averaged.

the quantum dot which are parallel to each other.

The cross section of the quantum dot with a certain fluctuating interface is shown in Fig.2(a). The interfaces fluctuate with the amplitude of $L/8$. We prepare ten potential patterns of fluctuating interfaces as shown in Fig.2(b). The periods of the fluctuation are L, $L/2$, and ∞ (without fluctuation). Note that the area where the potential exists is one half of each face of the quantum dot for all potential patterns. When the fluctuations of interfaces are averaged, the interface is uniformly shifted toward the inside by $L/16$ (as shown in Fig.2(c)) and the dimensions of the quantum dot become $L \times L \times \frac{7}{8}L$.

The finite element method is used to solve Eq.(1) numerically. We impose Dirichlet boundary condition $\psi(\mathbf{r}) = 0$ at the outer boundary of $Al_xGa_{1-x}As$. It is necessary to take the outer boundary as far as possible from the fluctuating interface. When $L' = 67.5$Å, the amplitude of the ground state wave function at outer boundary is less than 5% of that at interface for the potential of 0.2eV. This fact may justify our boundary condition in numerical analyses.

3. RESULTS

We obtain the ground state eigenvalues and wave functions with fluctuating interfaces of ten patterns and without fluctuation. In Fig.3, we plot the results for band offset of 0.2eV as ratios to the eigenvalue without fluctuation. The volume of well part is $L \times L \times \frac{7}{8}L$ in all cases with and without fluctuation. Eigenvalues with fluctuation, however, are generally larger than that without fluctuation.

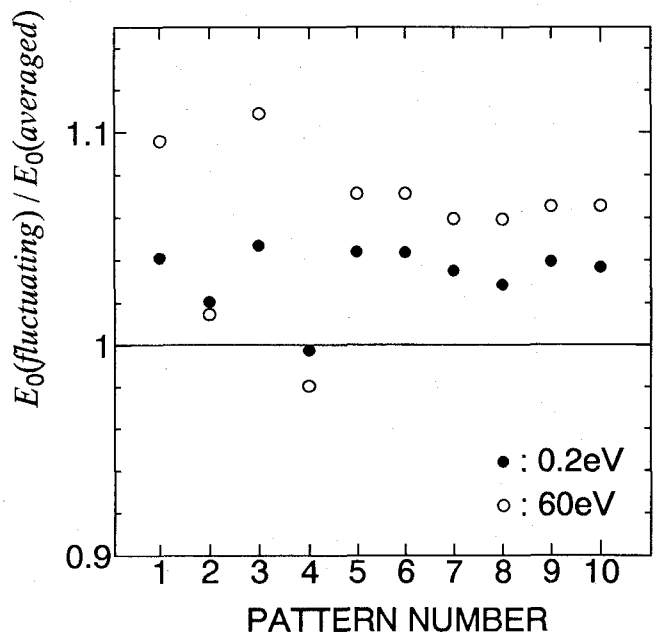

Fig.3. Ground state energy eigenvalues with fluctuating interfaces. These values are normalized by eigenvalue without fluctuation.

According to the uncertainty principle, the energy eigenvalue increases when the domain confining a particle decreases. This result thus indicates that, when the fluctuation exists at the interface of the quantum dot, the effective volume of confinement decreases compared with the real volume of low potential part.

The wave functions for fluctuations with patterns 5 and 6 are shown in Fig.4(a), in comparison with the case without fluctuation. The interfaces corresponding to these wave functions are shown in Figs.4(c), (d), and (e). We see that the wave functions with fluctuating interfaces (two kinds of broken lines) are deformed by fluctuations. The deformation, however, does not follow exactly the profile of interface and the electron is effectively confined in smaller volume compared with the smooth interface (dotted line).

Let us denote the period or the wavelength of the fluctuation of interface by λ_f and discuss the relation between λ_f and the effective volume of confinement. Without fluctuation, the ground state eigenvalue in the quantum dot of the size $L \times L \times (\frac{7}{8}L - 2x)$ is plotted in Fig.5. We also plot the value for the case where λ_f is $L/2$ (patterns 5 and 6) with a broken line. This figure shows when $\lambda_f = L/2$, x is about 60% of $L/16$. The effective volume of confinement is reduced to 91% of the real volume due to the fluctuation.

If $\lambda_f \to 0$, x is expected to become $L/16$ since the wave function cannot follow the fluctuation: The characteristic length of deformation of the ground state wave function λ_w may be estimated as $2L$ and when $\lambda_f \ll \lambda_w$, the fluctuation of interface may be equivalent to the existence of advanced interfaces. The effective volume is thus expected to decrease further when λ_f becomes smaller than $L/2$. The present data, however, do not allow us to determine this dependence on λ_f.

When we impose the fluctuating interfaces with patterns 5 and 6 on two and three parallel pairs of faces of the quantum dot, the results show that the consequence of two parallel interfaces can be applied also to these cases. For example, when we express the ground state eigenvalue with fluctuation on two parallel pairs of interfaces by that of $L\times(\frac{7}{8}L-2x)\times(\frac{7}{8}L-2x)$ quantum dot without fluctuation, x is estimated to be also about 60% of $L/16$.

We now take the conduction band offset of 60eV and make a similar analysis. In this case, the potential may be regarded as ∞ since it is high enough compared to the ground state eigenvalues ($\sim$0.2eV). We show the results in Figs.3 and 6. The eigenvalues for profiles $5 \sim 10$ tend to shift uniformly compared with the case where the potential is 0.2eV and we estimate x to be about 60% of $L/16$ for patterns 5 and 6. These results indicate that the effective volume of confinement is independent of the height of the conduction band offset when the fluctuation has the wavelength $\lambda_f = L/2$.

In conclusion, we have analyzed the ground state eigenvalues of cubical quantum dots with fluctuating interfaces and have shown that the effective volume confining electrons becomes substantially smaller than the real volume of well part due to the effect of fluctuations.

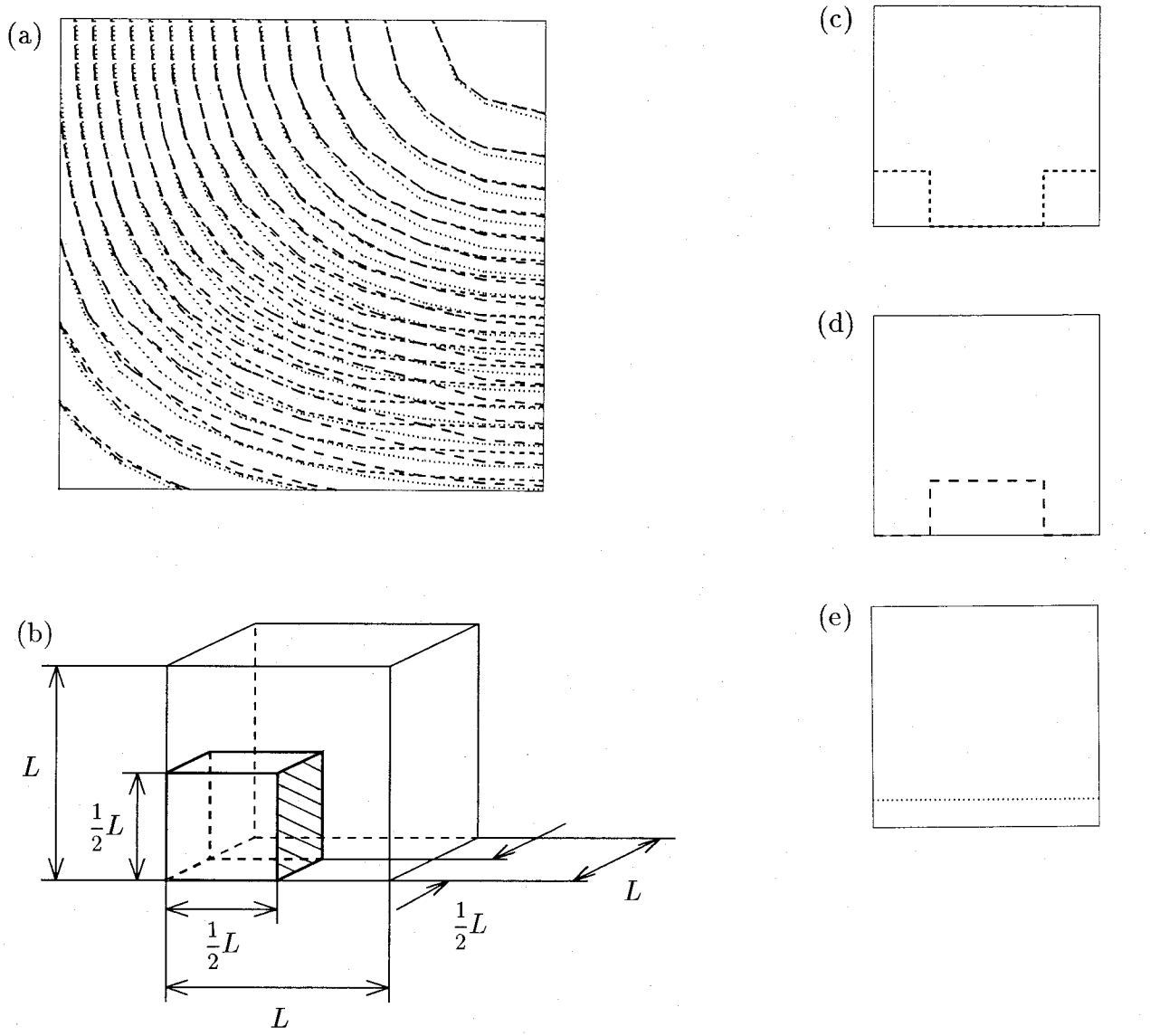

Fig.4. (a)Contours of wave functions for three kinds of interfaces. (b)Contours are taken in hatched area. (c)~(e)Interface profiles corresponding to patterns 5(c), 6(d), and smooth interface(e). Types of lines correspond to contours in (a).

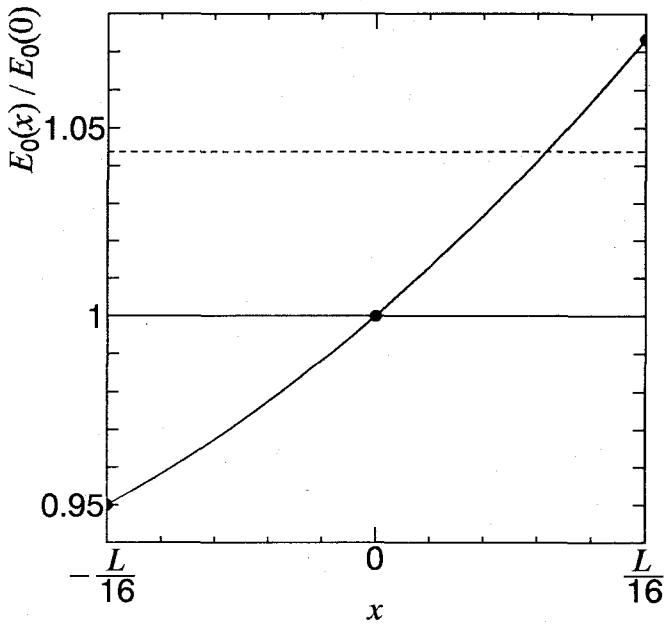

Fig.5. Energy eigenvalue without fluctuation E_0. Dimensions of quantum dot are $L \times L \times (\frac{7}{8}L - 2x)$. Results for patterns 5 and 6 are shown by dotted line. Height of barrier is 0.2eV.

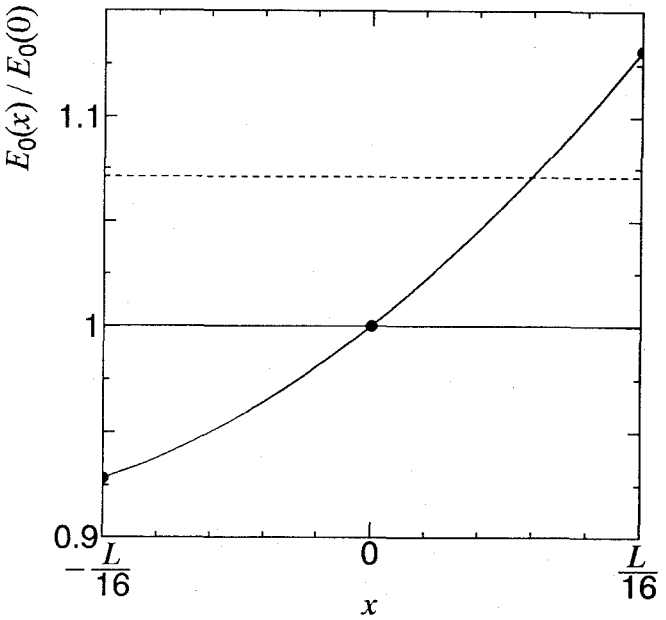

Fig.6. Same as Fig.5. Height of barrier is 60eV.

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