Analysis of the Vertical and Lateral Interactions in a Multisheet Array of InAs/GaAs Quantum Dots

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The vertical and lateral interactions in a multisheet array of InAs/GaAs quantum dots are analyzed by finite element method (FEM). It is shown that due to the effects of vertical interaction, nucleation prefers to happen above buried quantum dots (QDs). Mearwhile, the effects of lateral interaction adjust the spacing of lateral neighboring QDs. The vertical coupling becomes strong with deceasing GaAs spacer height and increasing number of buried layers, while the lateral coupling becomes strong with increasing InAs wetting layer thickness. The phenomenon that, after successive layers, the spacing and size of QDs islands become progressively more uniform is explained according to the minimum potential energy theory.

KEY WORDS: Quantum dots; Vertical and lateral interactions; Finite element analysis

1. Introduction

The particular optical and electronic behaviors of zero-dimensional nanostructure have aroused great interest in recent years. Quantum dots (QDs) become fascinating objects because of their successful application in laser, detectors and other electronic devices. An effective way to grow QDs is by depositing a thin film of material on a substrate. As the result of competition between strain energy and surface energy, the two-dimensional-three-dimensional transition (*i.e.* island formation) occurs at a critical deposited layer thickness[1–4]. The self-assemble growth mode of QDs is known as Stranski-Krastanow (SK) growth.

In order to integrate QDs into semiconductor industry, the technique of obtaining uniform island size and spacing becomes important. An interesting hybrid structure is to grow multiple layers of the heterostructure to form QD superlattices. Figure 1 presents uncapped conical surface InAs/GaAs QDs sitting on multiple layers of buried QDs. Due to the close spatial and optical correlation between surface and buried QDs, the photoluminescence emission from surface QDs is significantly improved. It is shown that surface QDs have great potential for sensing biological agents[5]. So, forming ordered QD island arrays using strain patterning by embedded inclusions in the substrate provides a good solution for practical application.

Researches on self-organization in the growth of QDs superlattices revealed that surface QDs do more than just mimic the arrangement in the layers below. The island sizes and spacing actually become more regular with each successive layer[6]. In this work, the finite element code FEAP (copyright by R.L. Taylor at U.C. Berkeley and J.C. Simo at Stanford University) is employed to provide the simulations given in this paper. We shall show how and to what extent the neighboring QDs, including buried QDs and lateral nearest QDs, affect the strain and stress fields in surface QDs. The number of buried QD layers, the thickness of GaAs spacer and InAs wetting layer play important roles in the coupling effects of multilayered QDs structure.

2. Finite Element (FE) Analysis

The QDs system is much more than 1000 atoms, so it can be well described by continuum elasticity theory. According to the minimum potential energy theory, the variation of the total potential energy, Π, vanishes, *i.e.*

$$\delta\Pi = \delta(U_\mathrm{e} - V) = 0 \tag{1}$$

where V is the work done by all external forces. The volume strain energy, U_e, is given by

$$U_\mathrm{e} = \int_{B_i} \sigma \mathrm{d}\varepsilon = \int_{\mathrm{B_i}} \Big(\frac{1}{2}\varepsilon^\mathrm{T} D\varepsilon - \varepsilon^\mathrm{T} D\varepsilon_\mathrm{T}\Big)\Big)\mathrm{d}\Omega \tag{2}$$

where σ and ε are respectively body stress and strain, D denotes the material modulus matrix, ε_T is the thermal strain. Applying the isoparametric interpolations for displacement and coordination, a FE formulation can be developed.

The material properties of InAs and GaAs are shown in Table 1, and the lattice mismatch strain can be calculated as $\varepsilon_0=(a_\mathrm{GaAs} - a_\mathrm{InAs})/a_\mathrm{InAs}=-0.067$. In order to model the lattice mismatch, we simulated QD formation on strain-patterned epitaxial substrate in thermodynamics system. Set the thermal expansion coefficient α_T of InAs and GaAs as 0.067 and zero respectively, and raise the temperature of the system by 1 K. So the thermal expansion of InAs island is characterized by thermo strain $\varepsilon_\mathrm{T}=\alpha_\mathrm{T}\Delta T=0.067$. A "tied contact" condition was specified on the interface

Table 1 Material elastic properties and lattice parameters

Material	E/GPa	ν	Lattice parameter/nm
GaAs	86.92	0.31	0.564325
InAs	51.42	0.35	0.605830

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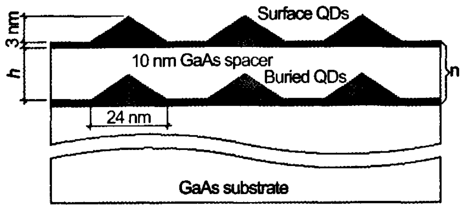

Fig. 1 Uncapped conical surface InAs/GaAs QDs sitting on multiple layers of buried QDs

edges between the InAs wetting layer and GaAs substrate.

2.1 Vertical interaction

Strain-driven self-organization of QDs on strain-patterned buried layers is under intense research both in experiment and theory[8–14]. For example, Quek and Liu[12] simulated the morphology of the quantum dot island due to stresses induced by a buried quantum dot. Wise *et al.*[9] and Liu *et al.*[13] studied anisotropy effect on QD formation on a strain-patterned epitaxial thin film. However, the variations in strain fields of surface QDs due to vertical interaction haven't been given quantitatively.

As shown in Fig. 1, the second and subsequent layers of QDs grow in the strain filed created by the buried QDs of the first layer. The effects of numbers of buried QDs layers (n) on the strain and through the center of surface QD island are shown in Fig. 2. It can be seen that the strains in surface QD are released greatly with one sheet of buried QDs layer (n=1). With deposition of the second sheet of the buried QDs layers (n=2), the strain energy is further released, but the variation is not as significant as previous. It is shown that the formation of island above buried QDs is energy favorable due to strain energy relaxation, which is explained by the maximum tensile stress on top surface of the cap layer above the center of buried QDs. According to the minimum potential energy theory, the equilibrium morphology is given by the lowest potential energy. So, nucleation prefers to happen according to the arrangement in the layers below, and the size of QDs becomes more uniform due to the simultaneous occurrence of nucleation. Furthermore, the effects of vertical interaction also depend on the distance between sheets. Figure 3 shows the influence of the thickness of GaAs spacer

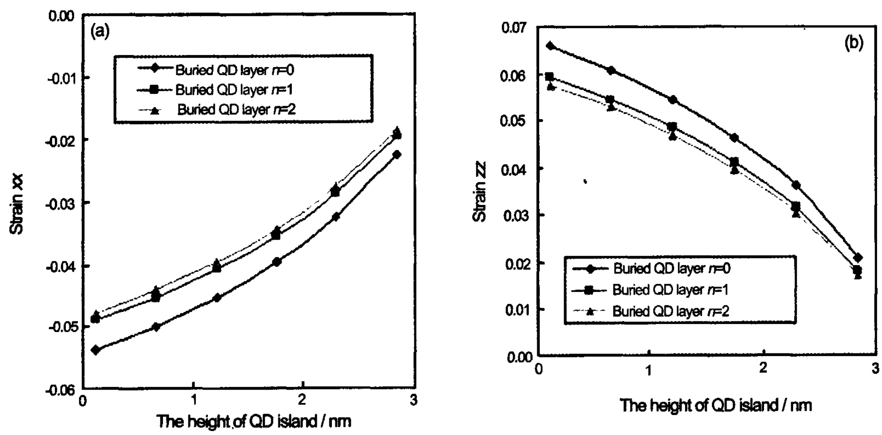

Fig. 2 Effects of numbers of buried QD layers (n) on the (a) strain and (b) strain along the center of surface conical QDs

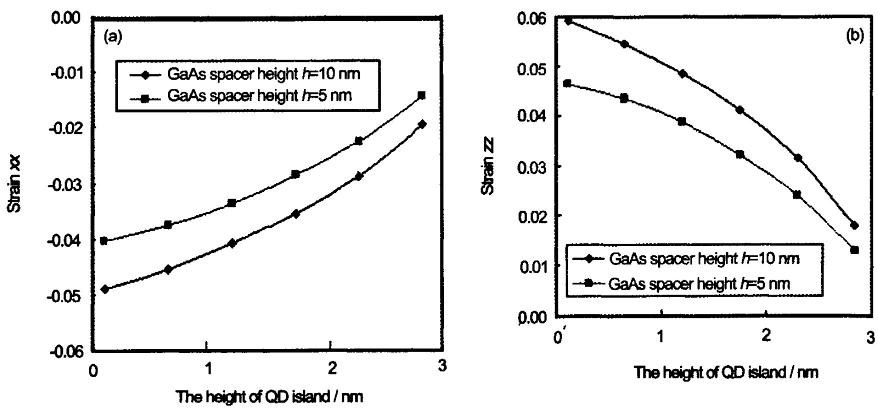

Fig. 3 Effects of GaAs spacer height on the (a) strain and (b) strain along the center of surface conical QDs

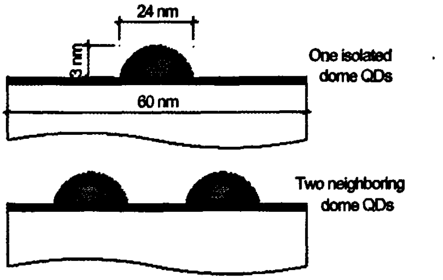

Fig. 4 One isolated dome QD and two closely neighboring dome QDs

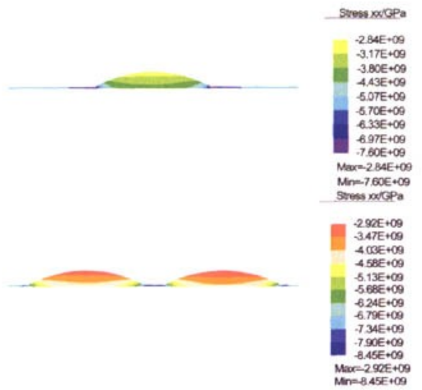

Fig. 5 Stress distribution of one isolated QD and two neighboring QDs

(h) on the strain fields of surface QDs. It is shown that the coupling between the surface QDs and buried QDs layer becomes strong with decreasing GaAs spacer height.

2.2 Lateral interaction

For technological applications, obtaining a high spatial density of QDs is essential. An alternative to get dense QDs matrix is to increase lattice mismatch[15]. In the case of dense QDs system, elastic interaction between islands *via* the substrate is accountable. FE results show the effects of lateral interaction on layers of conical, truncated or dome QDs are analogous. Here we analyze the strain and stress fields of one isolated dome QD and two closely neighboring dome QDs (shown in Fig. 4). We choose dome QDs model because dome is another common shape of QDs and previous works only analyzed conical and truncated QDs[2-4]. The strain and stress fields in dome islands are given to demonstrate the difference in dome, conical and truncated QDs. It should be mentioned that during the growth of QDs, conical shape is in favor of strain energy relaxation but with rather quickly increased surface free energy while dome QD is the mature and stable form of QD[16-17]. Boundary constrains are defined as follows: the nodes along the left and right boundary are constrained in the direction.

Figure 5 demonstrates the stress distribution of dome InAs/GaAs QDs. In contrast to the stress

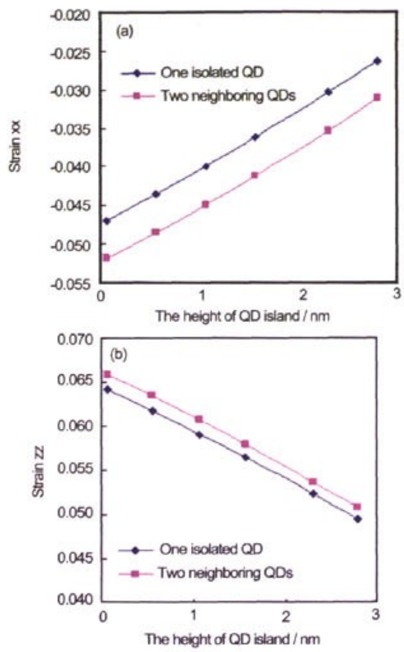

Fig. 6 Comparison of (a) strain and (b) strain through the center of one surface dome QD and two neighboring islands

fields of one isolated QD, We found that, with the lateral disturbance, the compressive stress σ_{xx} is intensified, leading to the increase in elastic strain energy. Besides, the lateral coupling becomes strong with increasing InAs wetting layer height. Comparison of strain and through the center of surface dome QD island is shown in Fig. 6. From them, we can also infer that lateral dense QDs are not in favor of strain energy relaxation. That corresponds with Ostwald ripening process. The process of ripening implies the coalescence of dense small islands into sparse large islands.

3. Conclusion

Because of vertical interaction, nucleation prefers to happen above buried QDs islands. That explains vertical alignment between islands in successive layers. Contrary to the effects of vertical interaction, the effects of lateral interaction cause an increment in elastic energy. The vertical coupling becomes strong with deceasing GaAs spacer height and increasing number of buried layers, while the lateral coupling becomes strong with increasing InAs wetting layer height. As the result of the competition of vertical and lateral interaction, the strain fields are gradually adjusted to find optimum position and spacing for surface QDs. It explains the phenomenon that, after successive layers, the size and spacing of QDs islands become progressively more uniform.

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