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Finite element analysis of conical, dome and truncated InAs quantum dots with consideration of surface effects

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Abstract
Surface effects on conical, dome and truncated InAs quantum dots (QDs) grown on GaAs (0 0 1) substrate are quantitatively analyzed with the finite element method (FEM) taking into account the surface energy. It is found that surface effects hinder island formation and arouse changes in strain fields of QDs. According to the minimum potential energy theory, the shape transition from conical island to dome island at a certain critical point is interpreted. We conclude that conical QD or truncated QD are transitional shapes at early stages while dome QD is the mature shape in this case.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Quantum dots (QDs) have recently attracted vast interest for potential use in the optoelectronic field due to their special optical and electronic properties. An effective way to grow dots is by depositing a thin film layer on substrate material, which is usually of a different material to the thin film. The growth mode of QD in the context of hetero-epitaxial growth is known as Stranski-Krastanow (SK), which comprises two kinds of growth: first, layer-by-layer growth mode (i.e. FvdM growth), and 3D island growth (i.e. VW growth) after a certain critical deposited thickness. The mechanisms of QD formation have been extensively studied (Kratzer *et al* 2006, Koo *et al* 2001, Wang *et al* 2000). Recent works state that the strain-driven spontaneous formation of QDs is a result of the combination of the lattice-mismatch-induced strain energy and the surface energy (Robin *et al* 2006).

Due to undercoordination, the atoms at the surface have extra energy than those in the bulk, and that is the source of surface energy. Surface energy, although small and negligible in conventional continuum mechanics, becomes significant in the growth of QDs. That is because of the high surface area to volume ratio, a particular feature for nanomaterials. The elastic energy, including both bulk and surface energy contribution, is the driving source responsible for ordering. It is generally believed that islanding happens due to the gain of elastic relaxation energy, but at the cost of increased surface energy. However, this is only a qualitative predication. In this work, we shall show how the surface energy influences the shape transition of QD. The calculation is based on the finite element method (FEM), considering surface energy.

The following approximations are made in this paper. (i) The influence of the edge energy is neglected because the contribution is rather small and the variation with QD volume is even smaller (Moll *et al* 1998). (ii) A 2D axi-symmetric model is used to model QD island shape in reality. It is feasible because FEM results show 2D model gives satisfactory results (Liu and Quek 2002, Benabbas *et al* 1999). (iii) Due to the 2D simplification, the surface elastic constant of various surface facets is assumed as a representative value. Further insight into 3D model shall be performed in our future work.

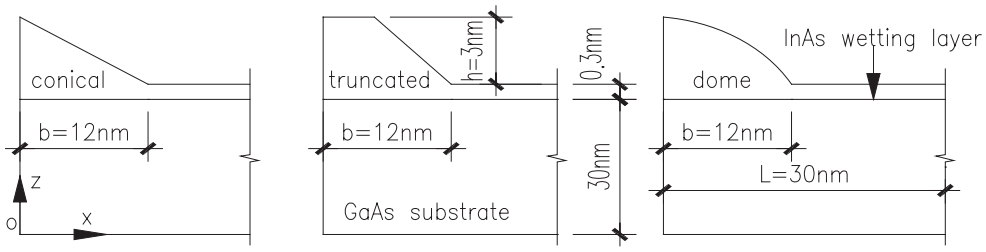

Figure 1. Conical, truncated and dome 2D axi-symmetric QD island.

2. Surface effects and finite element analysis

Surface effects on nanomaterials have become hot topics these years (Gao *et al* 2006, Dingreville *et al* 2005, Park *et al* 2006, Shenoy 2005, Wu 1999). As long as the QD island contains more than 1000 atoms, it can be well described by continuum theory (Moll *et al* 1998). We study surface InAs QD grown on GaAs (0 0 1) in the framework of thermodynamics. Thermodynamics of the surface stress σ_{ij}^s can be expressed by Shuttleworth's relation (1950) and Cammarata (1994) as

$$\sigma_{ij}^s = \frac{1}{A}\frac{\partial (A\gamma)}{\partial \varepsilon_{ij}^s} = \gamma\delta_{ij} + \frac{\partial \gamma}{\partial \varepsilon_{ij}^s}, \qquad (i, j = 1, 2) \tag{1}$$

where A is the surface area, γ is the surface energy, δ_{ij} is the Kronecker delta symbol and ε_{ij}^s is the surface strain. Analogous to equation (1), the surface stress is related to surface strain via (Miller and Shenoy 2000)

$$\sigma_{ij}^s = \sigma_{ij}^0 + S_{ijkl}\varepsilon_{kl}^s, \qquad (i, j, k, l = 1, 2) \tag{2}$$

where σ_{ij}^0 is the residual surface stress when the bulk is unstrained, and S_{ijkl} is the fourth order surface elastic constant which determines the change in the surface stress with strain. Their values can be determined from molecular dynamic simulation, such as the works of Shenoy (2005). Under two-dimensional conditions, the surface stress can be reduced to

$$\sigma^s = \sigma_0 + S\varepsilon^s. \tag{3}$$

Consider a thermo-elastic body which occupies domain B and surface domain $\hat{B}_i$. Taking into account the surface energy at surface domain $\hat{B}_i$, the total potential energy Π equals

$$\Pi = U_e + U_s - V, \tag{4}$$

where V is the work done by all external forces, U_e and U_s are respectively the volume elastic strain energy and the surface free energy. They are given by

$$U_e = \int_{B_i} \boldsymbol{\sigma}\, \mathrm{d}\varepsilon = \int_{B_i} \left(\frac{1}{2}\varepsilon^{\mathrm{T}}\mathbf{D}\boldsymbol{\varepsilon} - \varepsilon^{\mathrm{T}}\mathbf{D}\boldsymbol{\varepsilon}_{\mathrm{T}}\right) \mathrm{d}\Omega, \tag{5}$$

and

$$U_s = \int_{\hat{B}_i} \sigma^s\, \mathrm{d}\varepsilon^s = \int_{\hat{B}_i} \left[\gamma_0 + \sigma_0\varepsilon^s + \frac{1}{2}S\left(\varepsilon^s\right)^2\right] \mathrm{d}l, \tag{6}$$

where γ_0 is the unstrained constant surface energy, $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are respectively body stress and strain, $\mathbf{D}$ denotes the material modulus matrix and ε_{T} is the thermal strain. According to the minimum potential energy theory, the variation of functional Π vanishes, i.e. $\delta\Pi = 0$. Applying the isoparametric interpolations for displacement u and coordination x, a finite element formulation is developed as

$$(\mathbf{K}^{\mathrm{m}} + \mathbf{K}^{\mathrm{S}})\,\mathbf{d} = \mathbf{P} + \mathbf{P}^{\mathrm{T}} - \mathbf{P}^{\mathrm{S}}, \tag{7}$$

where $\mathbf{d}$ is the displacement vector of element nodes, $\mathbf{K}^{\mathrm{m}}$ and $\mathbf{K}^{\mathrm{S}}$ are respectively the material tangent matrix and the surface stiffness matrix, $\mathbf{P}$ is the external force vector, $\mathbf{P}^{\mathrm{T}}$ is the thermal stress vector and $\mathbf{P}^{\mathrm{S}}$ is the residual surface stress vector. The surface-energy-related terms are given as follows:

$$\left(K_{ij}^s\right)_{\mathrm{IJ}} = \sum_e \left[\int_{\hat{B}_i^e} S\frac{\mathrm{d}N_I}{\mathrm{d}l}\frac{\mathrm{d}x_i}{\mathrm{d}l}\frac{\mathrm{d}x_j}{\mathrm{d}l}\frac{\mathrm{d}N_J}{\mathrm{d}l}\mathrm{d}l\right], \tag{8}$$

$$\mathbf{P}^{\mathbf{S}} = \sum_e \left[\int_{\hat{B}_i^e} \sigma_0\frac{\mathrm{d}\mathbf{N}^{\mathbf{T}}}{\mathrm{d}l}\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}l}\mathrm{d}l\right], \tag{9}$$

where $\mathbf{N}$ is the shape function matrix, $\mathbf{N} = [\mathbf{N_1} \cdots \mathbf{N_I} \cdots \mathbf{N_n}]$, and

$$\mathbf{N_I} = \begin{bmatrix} N_I & 0 \\ 0 & N_I \end{bmatrix}.$$

Table 1. Material elastic properties and lattice parameters.

Material	E (GPa)	ν	Lattice parameter (Å)
GaAs	86.92	0.31	5.643 25
InAs	51.42	0.35	6.058 30

3. Conical, dome and truncated quantum dots

The typical shapes of InAs QDs grown on GaAs (0 0 1) can be well modeled by conical, dome or truncated 2D axi-symmetric islands as shown in figure 1 (Liu and Quek 2002, Benabbas *et al* 1999). Boundary constrains are defined as follows: the nodes along the $x = 0$ nm line and the $x = 30$ nm line are constrained in the x direction; a 'tied contact' condition is specified on the interface edges between the InAs QD and GaAs substrate. The material properties are shown in table 1, and the lattice mismatch strain can be calculated as $\varepsilon_0 = (a_{\mathrm{GaAs}} - a_{\mathrm{InAs}})/a_{\mathrm{InAs}} = -0.067$. Isotropic material properties are used, because 2D strain calculations, taking into account anisotropic behavior, show no significant effect (Moll *et al* 1998). In order to model the lattice mismatch, we set the thermal expansion coefficient α_{T} of InAs and GaAs as 0.067 and 0 respectively, and raise the temperature of the system by 1 K. So the thermal expansion of InAs island is characterized by thermo strain $\varepsilon_{\mathrm{T}} = \alpha_{\mathrm{T}}\Delta T = 0.067$. We consider the

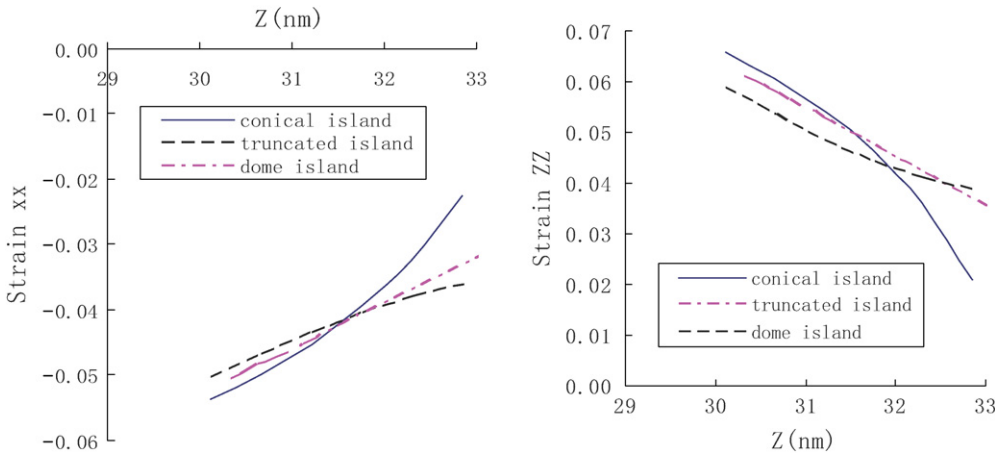

Figure 2. The strain ε_{xx} and strain ε_{zz} through the center of conical, truncated and dome QD islands.

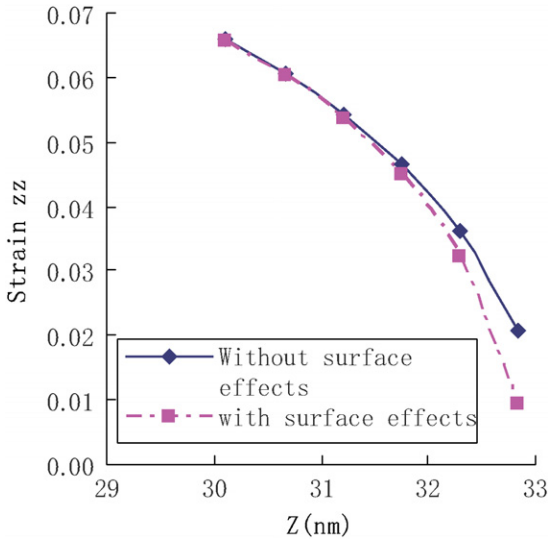

Figure 3. The variation of strain ε_{zz} through the center of conical QD island with and without consideration of surface effects.

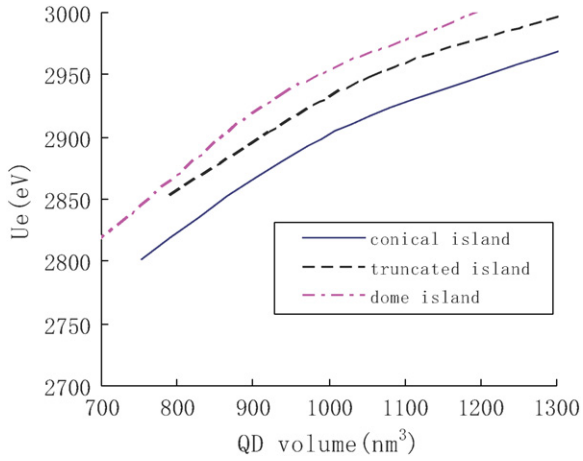

Figure 4. The dependence of QD island elastic strain energy U_e on the island volume.

surface energies for both the InAs island facets and the wetting layer, and set the surface elastic constant as $\gamma_0 = 42$ meV Å^{-2}, $\sigma_0 = 48$ meV Å^{-2} and $S = 125$ meV Å^{-2}.

Taking into account the surface energy, the strain fields of QDs analyzed with FEM are changed. We find that, induced by surface stress, the value of compressive strain ε_{xx} is exaggerated while the tensile strain ε_{zz} is reduced. It can be explained by the fact that surface stress always makes surface contract to reduce surface area. However, the changes in strain fields induced by surface effects rely on the QDs' shape greatly. The variation of strain ε_{zz} in conical island calculated with and without surface effects is shown in figure 2. For conical, dome and truncated QD islands with the same height-to-base ratio of 0.25 (i.e. $b = 12$ nm, $h = 3$ nm), the ε_{xx} and ε_{zz} strain through the center of the island are shown in figure 3. It is shown that the top of a conical island is more fully relaxed than the dome or truncated island and the flat top of a truncated island is not in favor of strain relaxation.

From the point view of thermodynamics, the optimum equilibrium shape of QD is given by the condition of lowest potential energy. Because surface effects try to hinder elastic deformation, the elastic strain energy of QD (including the wetting layer), U_e is found to be increased. For the given width of the island (i.e. $b = 12$ nm), the dependence of U_e on the island volume is shown in figure 4. From it, we can see, for a given volume, conical QDs relieve more elastic energy than the two other shapes. It also shows that a higher aspect ratio is energetically favorable due to more efficient strain relaxation in the steep part of the island (Kratzer *et al* 2006). That corresponds to the Ostwald ripening process. The process of ripening implies the growth of larger and taller islands at the expense of evaporation of small islands.

With the high surface-to-volume ratio, surface energy becomes accountable. For a given volume, the dome shape is that possessing minimum surface area. Besides, the surface energy U_s of the conical QD island facets increases most quickly with volume, followed by truncated island. Because the top region of a conical island is subjected to high surface stress concentration, it is possible to form the truncated island at an early stage. The sum of U_e and U_s is plotted in figure 5. It shows that the conical shape is energetically favorable for small

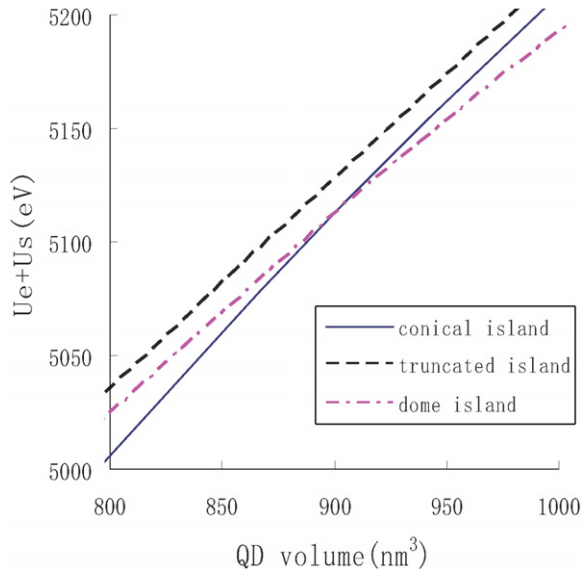

Figure 5. The dependence of the sum of U_e and U_s on the island volume.

island size. However, with island growth, shape transition from conical shape to dome shape will occur at a critical point. It agrees with phenomena observed in experiment which show conical shape is always observed at the beginning of island growth to be gradually replaced by domelike shaped larger and taller islands.

To conclude, the island is formed to gain relaxed strain energy. The role of surface stress is to hinder the island's growth and reduce the whole surface area. Considering surface stress, the strain field is altered in contrast to results obtained by conventional FEM. Furthermore, surface energy plays an important role in equilibrium shape transition. We found conical or truncated shape is preferable during the early stage of QD growth. With volume increasing, dome shape is more advantageous than conical shape or truncated shape at a certain shape transition point. Hence, large domelike-shaped island is the stable and mature form of QD.

Acknowledgments

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