Tuning and monitoring of quantum dot growth by an *in situ* **cantilever**

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Self-organization of quantum dots (QDs) on an *in situ* cantilever setup is investigated using a continuum approach. In this QD growth system, the cantilever has two functions. The first function is as a substrate of QD growth and the second is to tune and detect the morphologies of QDs. We calculate the free energy, consisting of elastic energy, surface energy, island-substrate interaction energy, wetting-layer-substrate interaction energy, and island-island interaction energy, and we analyze their contributions to the total free energy in the QD growth system. Then, we calculate the critical quantity of the deposited material, above which the QD growth system will transfer from the planar film state to the island array state, and the curvature of the cantilever during QD growth. The curvatures of the cantilever are functions of island coverage, island size, facet orientation of island, thickness of the wetting layer, and thickness of the cantilever. It is shown that the *in situ* cantilever setup can not only tune the morphologies of QDs by properly choosing the thickness of the cantilever but can also monitor the QD growth state with a high sensitivity.

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I. INTRODUCTION

Considerable experimental and theoretical interest has been paid to semiconductor quantum dots (QDs) due to the fact that quantum confinement offers a bright potential to improve the electronic and optical properties of the quantum dot devices[.1–](#page-6-1)[8](#page-6-2) Among the microelectronic fabrication techniques that produce QDs, the most widely used one is the self-organization method. $9-11$ $9-11$ The formation of QDs is a process in which the free energy of the system is minimized when QDs form. There are two growth stages of QDs, namely, the initial planar film state and the final island array state [i.e., the Volmer-Weber (VW) and the Stranski-Krastanow (SK) growth modes]. To understand the growth mechanisms it is desirable to have, at hand, measurement techniques for monitoring the growth processes *in situ* during deposition. There exist experimental techniques for monitoring the growth processes. For example, Floro *et al.*[12](#page-6-5) used the curvature-measurement technique for real-time stress determination. However, the curvature based on the Stoney equation in their work is only determined by the equivalent thickness of the deposited material and the thickness of the substrate; the morphology of QDs could not be monitored by curvature and was obtained by *ex situ* microscopy technique[.12](#page-6-5) It is noted that Hu *et al.* fabricated QDs in a molecular beam epitaxy (MBE) chamber equipped with an *in situ* cantilever measurement setup.^{13[,14](#page-6-7)} The cantilever in their setup has two functions. The first is as a substrate of QD growth and the second is as a sensor to detect the morphologies of QDs[.13](#page-6-6)[,14](#page-6-7) Miniaturization of a cantilever sensor can provide a very thin substrate on which QDs can be fabricated. Generally, the thinner the cantilever, the larger its deformation and sensitivity. The elastic deformation of the thin cantilever will influence the free energy of the QD growth system so as to influence the morphology of QDs.¹⁵ Therefore, the morphology of QDs can be tuned and monitored by changing the cantilever (substrate) thickness.

Generally, the free energy of the island array state (including substrate, wetting layer, and islands) consists of the elastic energies and surface energies of wetting layer and islands, the interaction energy between the substrate and wetting layer (and islands), and the interaction energy between the islands themselves. The interaction energies exist no matter how thick the substrate is. However, these interaction energies depend on the elastic deformation of the components (substrate, wetting layer, and islands) in the QD growth system. To the authors' knowledge, no study has taken into account these free-energy terms simultaneously and compared their contributions to the QD growth morphology, especially when the effect of substrate thickness is taken into account. For example, Chiu *et al.*^{[16](#page-6-9)} considered the contributions of the elastic energy and the wetting-layer (island)-substrate interaction energy to the free energy of the system but without the interaction energy between the islands themselves. Shchukin *et al.*[17](#page-6-10) considered the elastic self-relaxation and interaction energy between islands but without the surface energy and interaction energy between substrate and wetting layer (islands).

Among the theoretical models simulating the QD growth, there are two kinds of approximate method in treating the elastic energy of the substrate. The first is the rigid-substrate approximation,¹⁶ namely, there is no elastic deformation in the substrate and the only contribution to the elastic energy is from the wetting layer and islands. The second is the nonrigid-substrate approximation, namely, the elastic energy of the substrate contributes to the total free energy.¹⁸ In particular, Gill and $Cocks¹⁸$ treated the substrate as elastic half space, and the deformation of the substrate induced by the islands only exists beneath the island base. In their treatment, the free energy of the system with the elastic substrate can be determined from the energy of the equivalent system with the rigid substrate.

In this paper, we employ the elastic thin substrate (an *in* situ cantilever) to grow QDs so that it can be used to tune

FIG. 1. (Color online) (a) QD growth system consisting of substrate with finite thickness, wetting layer, and pyramidal QDs. (b) Representative volume element (RVE) of QD growth system.

and monitor the morphology of QDs during the growth process. A series of problems related to the self-organization of QDs on the *in situ* cantilever is investigated. We first calculate all the free-energy terms and compare their contributions to the total free energy when the substrate is thin. Then, we analyze the QD morphologies influenced by the substrate thickness. It is noted that when the substrate is thin and the elastic properties of the wetting layer and the substrate are very similar (e.g., the Ge/Si system), the deformation of the substrate cannot be neglected. Therefore, we take the nonrigid-substrate approximation, and the deformation of the substrate can be analytically determined by minimizing the total free energy. It is found that the curvature of the cantilever is a function of the island coverage, island size, facet orientation of the island, thicknesses of wetting layer and cantilever. Thus, the curvature will change with the evolution of the island morphology during the deposition process. The analysis of the curvature shows that the thin *in situ* cantilever setup cannot only tune the morphologies of QDs by properly choosing the thickness of the cantilever but can also monitor QD growth states with a high sensitivity. The present work provides a theoretical basis to guide the self-organization of QDs on the thin substrate.

II. FORMULATION

The growth of QDs is a kinetic process in which the deposited material is continuously deposited on the substrate. During this process, the deformation (extension and bending) of the substrate varies with the quantity of the deposited material. When the deposited material exceeds the critical quantity, the film will break up into islands. In this island array configuration, the deformation of the substrate will also be influenced by the evolution of the island morphology. If we assume that the deposition rate of material A is *R*, then the quantity of the deposited material is *Rt* at a specific time *t*. In the following, our investigation is in terms of the specific time *t* and we omit *t* for brevity.

Consider a system with substrate (material B with lattice parameter d_B and thickness h_s), wetting layer (material A with lattice constant d_A and thickness h_f), and pyramidal QDs [material A, height h_i , cf. Fig. $1(a)$ $1(a)$]. The strain in the substrate and in the wetting layer can be decomposed into a uniform extension component and a bending component. Letting c_0 be the extension strain component, κ as the curvature, and z_0 as the position of the neutral plane of the system [cf. Fig. $1(b)$ $1(b)$], then the strain in the substrate and in

the wetting layer will be $\varepsilon_s = c_0 + \kappa(z - z_0)$ and $\varepsilon_f = c_0 + \kappa(z)$ $-z_0$) + ε^* , respectively. ε^* is the mismatch strain between the wetting layer and substrate, which arises from the different lattice constants [defined as $\varepsilon^* = (d_A - d_B)/d_B$] and the thermal-expansion coefficients between the wetting layer and the substrate. To obtain simple analytical solutions, here we assume that the materials A and B are elastically isotropic. This assumption has been validated by comparing isotropic and anisotropic solutions for semiconductor materials.^{18[,19](#page-6-12)}

The mismatch strain between the wetting layer and the substrate results in strain energy in the system, which is the driving force for island formation. In addition to the strain energy, the free energy of the system is influenced by the wetting-layer-substrate interaction energy, island-substrate interaction energy, surface energies of the wetting layer and islands, and the island-island interaction energy. With refer-ence to Fig. [1,](#page-1-0) we investigate a RVE of area $D \times D$. At the specific deposition time *t*, the equivalent thickness of the material deposited on the substrate is *H* and the total volume of the deposited material on the RVE is *HD*² . We assume that the base size of the island is *L*, the facet orientation of the uniform island is φ , the island coverage is $q(=L^2/D^2)$, and the island height is $h_i = (L \tan \varphi)/2$. *H* is the sum of the thickness (h_f) of the wetting layer and the equivalent thickness (h_{eq}) of the islands. The equivalent thickness of the islands is obtained by the principle of equivalent volume, namely, let the volume of the pyramidal island be equal to that of the uniform film on the area $D \times D$, which leads to $h_{\text{eq}} = h_i L^2 / (3D^2)$.

The free energy of the QD growth system can be expressed as

$$
u = u_f + u_{\text{sub}} + u_{\text{is}},\tag{1}
$$

where u_f , u_{sub} , and u_{is} are the energies of wetting layer, substrate, and islands, respectively.

A. Energy of wetting layer (u_f)

The free energy of the wetting layer for the island array state includes the elastic energy, the interaction energy between the wetting layer and the substrate, and the surface energy of the wetting layer, i.e.,

$$
u_f = D^2 \int_0^{h_f} \left(\xi_{\rm FS} G_{\rm bin} + \frac{E_f}{1 - \nu_f} \varepsilon_f^2 \right) dz + D^2 \gamma_1 (1 - q) \tag{2}
$$

where G_{bin} is the interaction energy between the wetting layer and substrate, consisting of the long-range interaction (long-range van der Waals force) and the short-range inter-action (intermolecular force).^{[20](#page-6-13)} Although there are different kinds of expression of G_{bin} , their intrinsic physical essence is the same[.20](#page-6-13) For example, Chiu *et al.*[16](#page-6-9) modeled this interaction energy as a special type of film surface energy; while Daruka and Barabasi 21 simulated this interaction energy by the binding-energy method. Here, we employ the latter method, namely, the wetting-layer-substrate interaction is expressed as the binding energy. We will show in Table [I](#page-2-0) that the former method gave the same result as the latter one. The expression of G_{bin} in the binding-energy form is²¹

TABLE I. $(\Delta u_1 - \Delta u_0)/\Delta u_1$ varies with substrate thickness $\log_{10} h_s$ (h_s is normalized by 1 m, island size $L=6$ nm, island coverage $q=0.29$, and facet orientation of island $\varphi=11.5^{\circ}$).

$\log_{10} h_s$	-7.0	-6.0	-5.0	-4.0	Chiu et al. (Ref. 16)
$h_f = 1.0$ nm $(\Delta u_1 - \Delta u_0)/\Delta u_1$	0.2107	0.2108	0.2108	0.2108	0.1804
$h_f = 1.2$ nm $(\Delta u_1 - \Delta u_0)/\Delta u_1$	0.1430	0.1431	0.1431	0.1431	0.1339

$$
G_{\text{bin}} = \alpha \left[\Theta \left(\frac{z}{d_A} - 1 \right) e^{-(1/a)(z/d_A - 1)} + \Theta \left(1 - \frac{z}{d_A} \right) \right] - \Phi_{AA},\tag{3}
$$

where $\alpha = \Phi_{AA} - \Phi_{AB}$, $-\Phi_{AA}$ is the energy of an *AA* bond, $-\Phi_{AB}$ is the binding energy at the interface of the wetting layer and substrate, and $\alpha < 0$ is the wetting condition. Due to the short-range interactions, the binding energies of *A* atoms close to the substrate is modified. When we move from the interior of material A to the wetting-layer-substrate interface, the binding-energy density decreases from $-\Phi_{AA}$ to $-\Phi_{AB}$. $\Theta(m)$ is the Heaviside step function which is defined as $\Theta(m)=0$ if $m < 0$ and $\Theta(m)=1$ if $m > 0$. G_{bin} at $a \to 0$ corresponds to the absence of the short-range interaction. The coefficient ξ_{FS} in Eq. ([2](#page-1-1)) represents the contribution of wetting-layer-substrate interaction to u_f . $\xi_{FS}=0$ if we neglect this interaction, otherwise $\xi_{FS}=1$. The second term in the integration of Eq. (2) (2) (2) is the elastic energy of the wetting layer, where E_f and ν_f are the Young modulus and Poisson ratio of material A, respectively. The last term in Eq. ([2](#page-1-1)) is the surface energy of the wetting layer, and γ_1 is the isotropic surface energy density of the wetting layer.

B. Energy of substrate (u_{sub})

For the thin substrate, the island growth will induce the deformation of the substrate. Therefore, the elastic energy of the substrate will contribute to the free energy of the system. The elastic energy of the substrate has the similar expression as that for the wetting layer,

$$
u_{\rm sub} = D^2 \int_{-h_s}^{0} \frac{E_s \varepsilon_s^2}{1 - \nu_s} dz
$$
 (4)

where ε_s , E_s , and ν_s are the strain, the Young modulus, and Poisson ratio of the substrate, respectively. If the substrate thickness is very large, the deformation of the substrate is very small and u_{sub} approaches zero.

C. Energy of island (u_{is})

The free energy of the island contains the elastic energy of the island, the interaction energy between the island and the substrate, the island-island interaction energy, and the surface energy of the island,

$$
u_{is} = L^2 \int_{h_f}^{h_i + h_f} \left(\frac{E_f \varepsilon_i^2}{1 - \nu_f} + \xi_{IS} G_{bin} \right) \left(1 + \frac{h_f - z}{h_i} \right)^2 dz
$$

+
$$
\frac{L^2 \gamma}{\cos \varphi} + \xi_{II} u_{II}.
$$
 (5)

The integration term includes the elastic energy of the island

and the island-substrate interaction energy. They are obtained by integrating the elastic energy (or interaction energy) of a small element dF in the island [cf. Fig. [1](#page-1-0)(b)]. In the calculation of the island-substrate interaction energy, the element *dF* is treated as a wetting layer, and the interaction energy between dF and the substrate has the same expression as G_{bin} ^{[21](#page-6-14)} ξ_{IS} is a coefficient representing the contribution of islandsubstrate interaction energy to free energy. $\xi_{IS}=1$ if this interaction is considered, otherwise $\xi_{\text{IS}}=0$. The second term is the surface energy of the island, where γ is the isotropic surface energy density of the island. u_{II} in the last term is the island-island interaction energy, which is calculated in terms of the dipole-dipole approximation in the case where the distance between the two islands is much larger than the lateral size of the island.²² Noting that when the substrate is thin, the interaction between islands becomes important via the strained substrate. Therefore, the island-island interaction energy (u_{II}) can be expressed as $u_{\text{II}} = L^3 E_f \epsilon_i^2 (h_f) q^{3/2} g(\varphi)$, $g(\varphi)$ is a function of facet orientation corresponding to the geometry of the island.²² Here, ξ_{II} has the similar definition to ξ_{IS} , but it stands for the contribution of the island-island interaction energy to the free energy. The contribution of u_{II} to the total free energy will be shown in the numerical result.

The total free energy of the system can be obtained by combining Eqs. ([2](#page-1-1))–([5](#page-2-1)), and it is a function of c_0 , κ , and z_0 . We minimize the total free energy with respect to c_0 , κ , and $z₀$, and we get three equations about them. The analytical solutions of $c_0(h_s, h_f, h_i, L, q)$, $\kappa(h_s, h_f, h_i, L, q)$, and $z_0(h_s, h_f, h_i, L, q)$ can be obtained by solving these three equations. For brevity, we do not show their lengthy expressions. Generally, in the QD growth system, the equivalent thickness of the deposited material is much smaller than the thickness of the substrate. In this case, the extension strain c_0 is much smaller than the bending strain $\kappa(z-z_0)$. Therefore, we will neglect the extension in the following calculation. By substituting the solutions of κ and z_0 into Eq. ([1](#page-1-2)), the free energy of the system can be obtained. It is noted that when h_s is very large, the deformation of the substrate is so small that it can be neglected. This proves that the semi-infinite substrate approximation is proper when the substrate is very thick.

The free energy of the initial planar film state (consisting of wetting layer and substrate) is composed of the elastic energy and the surface energy of the wetting layer, the elastic energy of the substrate, and the wetting-layer-substrate interaction energy, namely, $u_{\text{in}}(H, h_s, \varepsilon^*) = u_f^* + u_{\text{sub}}$, where u_f^* is the energy of the uniform wetting layer, which can be obtained by letting $q \rightarrow 0$ and $h_f \rightarrow H$ in Eq. ([2](#page-1-1)), and the expression of u_{sub} is the same as Eq. ([4](#page-2-2)). When the system transfers from the planar film state to the island array state, the difference of the free energy between these two states is $\Delta u = u$

FIG. 2. (Color online) Variation in the critical thickness H_{cr} of wetting layer with a substrate thickness of *hs*.

 $-u_{\text{in}}$. $\Delta u = 0$ is the critical condition between the two states.

In the following, we will show how the substrate thickness affects the total free energy and how the substrate thickness can be used to tune and monitor the quantum dot growth. We will consider the InAs (A, wetting layer)/GaAs $(B,$ substrate) system. The mismatch strain of InAs/GaAs is ε^* =0.07. For simplification, Δu is normalized by γd_A^2 in the following numerical evaluation.

III. CONTRIBUTIONS OF FREE-ENERGY TERMS

When the material is deposited on the substrate, it will be in the planar film state initially, and the deposited material totally contributes to the wetting layer (planar film). If the thickness of the wetting layer exceeds a critical value (H_{cr}) , it will break up into island array in self-organization process, and then the deposited material contributes to the wetting layer and the islands. The critical thickness of the wetting layer is defined by $\Delta u|_{H=H_{cr}} = 0$. When $H < H_{cr}$ and $\Delta u > 0$, the system will be in the initial planar state. As the deposition process continues, when the thickness of the wetting layer exceeds the critical value (H_{cr}) , the system will transform from the initial state $(\Delta u > 0)$ to the island array state $(\Delta u < 0)$. Figure [2](#page-3-0) shows the variation in H_{cr} with the thickness h_s of the substrate. Here, we assume that the equivalent thickness (h_{eq}) of the initial formed island is very small compared to the total deposited material $(h_{eq}/H \sim 0.03-0.04)$. It can be seen that H_{cr} decreases with the decrease in the substrate thickness, e.g., $H_{cr}=0.8$ nm at $h_s=0.1$ μ m and H_{cr} =1.0 nm at h_s =1 μ m. Therefore, when the substrate is thin, the deposited material is much easier to break up into islands. Moreover, when the substrate is thicker than h_s $=10$ μ m, the critical thickness of the wetting layer, namely, the critical thickness of the deposited material, will not be influenced by the substrate thickness (cf. Fig. [2](#page-3-0)). As mentioned in Sec. I, Hu *et al.*^{[13](#page-6-6)[,14](#page-6-7)} fabricated QDs in a MBE chamber equipped with an *in situ* cantilever measurement setup. In their experiment, InAs is deposited on a GaAs (001) substrate with thickness $h_s = 150 \mu$ m. By using the present theory, we get $H_{cr}=1.01$ nm, which agrees with the result in their experiment. This proves the rationality of the present theoretical model.

FIG. 3. (Color online) Ratio of island-island interaction energy u_{II} to Δu as a function of island coverage *q* (the thickness of wetting layer is h_f =1.2 nm, island size is $L=3$ nm, and facet orientation of island is $\varphi = 11.5^{\circ}$).

Table [I](#page-2-0) shows the contributions of the island-substrate interaction energy and wetting-layer-substrate interaction energy to the total free energy. We define two parameters Δu_0 and Δu_1 , i.e., $\Delta u_0 = \Delta u \big|_{\xi_{FS} = \xi_{IS} = 0, \xi_{II} = 0}$ and Δu_1 $=\Delta u|_{\xi_{\text{FS}}=\xi_{\text{IS}}=1, \xi_{\text{II}}=0}$. Therefore, the ratio of wetting-layersubstrate interaction energy and island-substrate interaction energy to the total free energy can be expressed as (Δu_1) $-\Delta u_0$) / Δu_1 . We choose two values of wetting-layer thickness $(h_f = 1.0$ and 1.2 nm) to illustrate the contributions of wetting-layer-substrate interaction and island-substrate interaction to the total free energy. Note that in Table [I](#page-2-0) the chosen deposited material thickness, consisting of the wetting-layer thickness $(h_f = 1.0 \text{ and } 1.2 \text{ nm})$ and the equivalent thickness of the island $(h_{eq} = 0.06 \text{ nm})$, exceeds the critical thickness (H_{cr}) which can be seen in Fig. [2.](#page-3-0) Table [I](#page-2-0) shows that the ratio $[(\Delta u_1 - \Delta u_0)/\Delta u_1]$ is large for both of the wetting-layer thicknesses $(h_f = 1.0 \text{ and } 1.2 \text{ nm})$. Therefore, the contributions of these interactions cannot be neglected; they should be taken into account in the QD growth process. It is noted that Chiu *et al.*[16](#page-6-9) also considered the island-substrate interaction and wetting-layer-substrate interaction by modeling them as a special kind of surface energy when the substrate thickness is infinite. The last column in Table [I](#page-2-0) shows the value of $(\Delta u_1 - \Delta u_0) / \Delta u_1$ in their paper. It can be seen that when the substrate thickness is 100 μ m, the contributions of these two interactions to the free energy in our model approach those in the paper of Chiu *et al.*[16](#page-6-9) Moreover, the island-substrate interaction energy and wetting-layersubstrate interaction energy favor the formation of island (cf. Table [I](#page-2-0)).

Figure [3](#page-3-1) shows the ratio $(u_{\text{II}}/\Delta u)$ of island-island interaction energy (u_{II}) to Δu at different island coverage *q* and substrate thickness h_s . $u_{\text{II}}/\Delta u$ increases with the increase in *q* and h_s . u_{II} becomes important especially when the island coverage is large. In the present analysis, the island-island interaction energy is calculated by the dipole-dipole approximation, which is the long-range interaction from a physical point of view. Shchukin *et al.*[17](#page-6-10) considered the short-range interaction between islands when the island array is very dense and found that the short-range interaction between is-

FIG. 4. (Color online) Contour of Δu varies with island coverage *q* and substrate thickness h_s (the thickness of wetting layer is h_f =1.2 nm, island size is $L=6$ nm, and facet orientation of island is $\varphi = 11.5^{\circ}$).

lands is important when the coverage of the islands is above 0.88. Therefore, the dipole-dipole approximation used to calculate the island-island interaction energy is appropriate when the island array is not very dense. The value of u_{II} in Fig. [3](#page-3-1) shows that the island-island interaction favors the planar film state. From the analysis of Table [I](#page-2-0) and Fig. [3,](#page-3-1) we know that the wetting-layer-substrate interaction energy, island-substrate interaction energy, and the island-island interaction energy are important in the QD growth process. Therefore, they should be taken into account in simulating the QD growth process.

IV. TUNING OF MORPHOLOGICAL EVOLUTION OF QDS

Now, we evaluate how the substrate thickness affects Δu and thereby tunes the morphology of QDs. Figure [4](#page-4-0) shows the contour of Δu when island coverage q and substrate thickness h_s vary. As seen from Fig. [4,](#page-4-0) Δu can be positive or negative by adjusting h_s and q . The zone with blue dash lines represents $\Delta u \leq 0$, and the zone with green solid lines represents $\Delta u > 0$. The black line, which is the dividing line between the two zones with $\Delta u < 0$ and $\Delta u > 0$, represents $\Delta u=0$. $\Delta u=0$ is the critical condition for the transition between the initial planar film state and island array state. When $\Delta u < 0$, the system is in the island array state. It is seen from Fig. [4](#page-4-0) that the substrate thickness has a great effect on the state of the QD system. When $h_s > 1$ μ m, the value of Δu is almost not influenced by the substrate thickness. However, when h_s <1 μ m, the value of Δu is much influenced by the substrate thickness. The thinner the substrate, the larger the island coverage for the island array. Therefore, the system with a thin substrate can have a different QD morphology from that with a thick substrate. The substrate thickness can be used as a parameter to tune the morphologies of QDs.

Figure [5](#page-4-1) shows the variation in Δu with island size *L*. As shown in Fig. [5,](#page-4-1) there exists a global minimum of Δu among the island array state of QDs $(\Delta u < 0)$ for a fixed island

FIG. 5. (Color online) Variation in Δu with island size *L* (the thickness of wetting layer is $h_f = 1.2$ nm and facet orientation of island is $\varphi = 11.5^{\circ}$).

coverage and substrate thickness. L_{cr} and L_{st} are the critical and stable sizes of QDs, which are defined by $\Delta u|_{L=L_{cr}}=0$ and $\frac{\partial (\Delta u)}{\partial L}|_{L=L_{\text{st}}}=0$, respectively. Moreover, at the same island coverage $q=0.1$, by comparing the critical and stable island sizes at different substrate thicknesses (e.g., $h_s=0.1$ and 10 μ m), we can know that L_{cr} and L_{st} are smaller when the substrate thickness is smaller. Therefore, the substrate thickness has an influence on the stable island size and can be used to tune the size of QDs. Moreover, at the same substrate thickness $(h_s = 0.1 \mu m)$, the stable island size decreases with the increase in island coverage. This finding was qualitatively proved by the research work of Hu .¹³

V. MONITORING OF MORPHOLOGICAL EVOLUTION OF QDS

During the deposition process, the curvature $\kappa(t)$ of the cantilever depends on the growth states of QDs. When the deposited material exceeds the critical thickness, the initial planar film will break up into island array. If the deposited process continues, the subsequent deposited material will contribute to the formation of island, and the corresponding curvature will also change with the state of system. Figure [6](#page-5-0) shows the variation in curvature $\kappa(t)$ with the thickness of deposited material $H(t)$. From the research work of Hu,¹³ we know that the deposition rate of material A is *R* $=0.01$ nm/*s* and $H(t) = 0.01t$. Therefore, Fig. [6](#page-5-0) actually shows the variation in curvature $\kappa(t)$ with the deposition time *t*. Note that in Fig. [6,](#page-5-0) we assume that the newly deposited material only contributes to the island sizes, but island coverage remains $q=0.2$ during the growth process of island. This assumption agrees with $Hu's^{13}$ experiment. It can be seen from Fig. [6](#page-5-0) that the slope of the curvature shifts at H_{cr} , which means that κ shifts when the state transition happens. For the same substrate $(t_s = 0.1 \mu m)$, when the orientation of the island is different (e.g., $\varphi = 11.5^{\circ}$ and $\varphi = 10^{\circ}$), the slope of the curvature is also different. Therefore, the measurement of curvature can be used to monitor the growth state of QDs. Moreover, the smaller the substrate thickness, the larger the

FIG. 6. (Color online) Variation in curvature κ with the equivalent thickness *H* of the deposited material.

curvature of the cantilever (cf. Fig. 6). In the following, we will give a detailed description about how the substrate thickness will influence the curvature of the cantilever.

Figure [7](#page-5-1) shows the variation in curvature κ with $log_{10}(h_s/h_f)$. It is shown that the curvature does not change monotonously, and there exists a critical point of the curvature at a specific value of h_s/h_f . Below this critical value, the curvature increases with the increase in h_s/h_f ; above this critical value, the curvature decreases with the increase in h_s/h_f . It should be noted that when h_s and h_f are in comparative order, the extension strain c_0 becomes important. We plot two curvatures with and without extensions in Fig. [7](#page-5-1) and find that the extension strain c_0 should be taken into account when $h_s \leq h_f$. Moreover, it is seen that the curvature is very large when the thickness of the substrate is small. These phenomena with a large curvature and a critical point have been proved by an experiment in terms of InGaAs/GaAs bilayers on a substrate. 23 In the experiment, when the two layers are both thin enough they will roll up into nanotube by self-organization. For example, when a GaAs film with a thickness of 20.4 MLs $(h_s/h_f = 0.069)$ or 6.4 MLs (h_s/h_f) $=0.22$) was deposited onto an ultrathin InAs substrate with a thickness of 1.4 MLs, the diameters of the nanotubes are 550 and 35 nm, respectively. It was found from this experiment that the bending curvature increases (the diameters of nanotube decreases) with the increase in h_s/h_f , which is the same as that (the part before the critical point) in Fig. 7 . The curvature with the large value (can be as high as $10^{15}/m$) was also confirmed by Huang *et al.*^{[24](#page-6-17)} for an ultrathin substrate with $h_s = 1$ μ m.

The strain in the substrate is defined as $\varepsilon_s = c_0 + \kappa(z - z_0)$. From the calculation, we know that the strain at the upper surface $(z=0)$ of the substrate is larger $(\varepsilon_s = -4.0 \times 10^{-3})$ for a thin substrate $(h_s = 0.1 \mu m)$ than that $(\varepsilon_s = -4.2 \times 10^{-5})$ for a thick substrate $(h_s = 10 \mu m)$. Further, for a substrate with thickness $h_s = 0.1$ mm, the strain can even be as small as ε_s $=-4.2\times10^{-6}$. Therefore, the elastic energy of the substrate is small when the substrate is thick, which shows the rationality

FIG. 7. (Color online) Variation in curvature κ with h_s/h_f (the thickness of wetting layer is $h_f = 1.2$ nm, island size is $L = 6$ nm, island coverage is $q=0.1$, and facet orientation of island is φ $=11.5^{\circ}$).

of the semi-infinite substrate approximation in some previous works. Moreover, Hu^{13} measured the stress evolution during InAs wetting-layer growth on the GaAs substrate (an *in situ* cantilever) when the deposition process took place at a temperature of 470 °C and the elastic constants of InAs are c_{1111} =80 GPa and c_{1122} =45 GPa. By using the present theoretical model, we obtain a stress in the wetting layer of 5.2 GPa, which is close to 4.7 GPa in $Hu's^{13}$ experiment. In her experiment, the substrate thickness is 150 μ m and the corresponding curvature calculated by our model is 0.03/m (cf. Fig. [7](#page-5-1)). If the substrate thickness is further decreased (e.g., $h_s = 1.2 \sim 120 \mu m$, cf. the inset of Fig. [7](#page-5-1)), the curvature of the cantilever will be much higher, and the corresponding sensitivity of the cantilever will be largely increased.

VI. CONCLUSIONS

We have proven that the morphology of QDs can be tuned and monitored by the *in situ* cantilever if its thickness can be properly chosen. By comparing the contributions of freeenergy terms, it is shown that the elastic energy, surface energy, island-substrate interaction energy, wetting-layersubstrate interaction energy, and island-island interaction energy are very important in controlling the morphology of QDs growth, especially when the thickness of the substrate is thin. The present work provides a theoretical basis to guide the self-organization of QDs on the thin substrate.

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