Morphological evolution of heteroepitaxial islands during Stranski–Krastonov growth

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Abstract

Three-dimensional finite element method is used to simulate the formation, self-assembly and shape transition of heteroepitaxial islands during Stranski–Krastonov growth. In the formulation, strain energy, surface energy, surface anisotropy and elastic anisotropy of a cubic lattice structure are taken into account. In the simulations, the SiGe/Si material system is used as a model system. An empirical surface energy as a function of surface orientation is proposed. The minimum energy surfaces are identified based on existing experimental observations. The simulation results show that the coupling of elastic energy relaxation, surface energy anisotropy and elastic anisotropy strongly influences the surface roughening morphology, self-assembly and shape transition of epitaxial islands, resulting in diverse evolution pathways.

Keywords: Epitaxial islands; Surface diffusion; Finite elements; Self-assembly

1. Introduction

Much attention has been paid to the study of heteroepitaxial growth of self-organized quantum dots. The main objective is to develop quantum dot-based nanoelectronic devices (Drucker, 2002; Baribeau et al., 2005). For these applications, uniform and regular arrays of quantum dot are often required. Although enormous experimental (Floro et al., 1998; Chaparro et al., 2000; Vailionis et al., 2000; Jesson et al., 1996; Ross et al., 1999; Medeiros-Ribeiro et al., 1998), modeling and simulation (Obayashi and Shintani, 1998; Zhang and Bower, 2001; Tersoff et al., 2002; Eisenberg and Kandel, 2005; Golovin et al., 2003, 2004; Shchukin et al., 1995; Guyer and Voorhees, 1995; Spencer and Tersoff, 1997; Johnson and Freund, 1997; Baribeau et al., 2006) effort has been made to achieve this task, there are many unresolved issues regarding the kinetics and thermodynamics underlying the quantum dot formation and self-assembly. Ge and SiGe on Si(001) or InGaAs on GaN(001) systems have been commonly used as a model system for understanding these issues.
However, even in these seemingly simple systems, the epitaxial processes are proved to be extremely complex (Tersoff et al., 2002).

The surface roughening process and its subsequent island formation can be understood by a simplified energetic argument (Srolovitz, 1989; Gao and Nix, 1999; Johnson and Freund, 1997), the total strain energy of the thin film system decreases while the surface total energy increases. For a perturbed wavelength \( \lambda \) in an isotropic film and substrate, when \( \lambda > \lambda_{\text{cr}} \), where \( \lambda_{\text{cr}} \) is the critical wavelength depending on the surface energy and strain energy density of the initially flat film, surface roughening is energetically favorable. However, when \( \lambda < \lambda_{\text{cr}} \), the perturbation will disappear and the surface will remain flat. When the surface energy anisotropy and elastic anisotropy are included, the critical wavelength may change with the elastic and surface energy anisotropies. Thus tuning these anisotropy strengths will change the roughening kinetics and therefore affect the island morphology.

Experimental observations have demonstrated the strong effect of surface energy anisotropy on surface morphologies of epitaxial growth. For example, strong energy anisotropy constrains island height, resulting in the quantum wire formation, that is, the square-to-rectangular island-base transition (Tersoff and Tromp, 1993). In addition, during SiGe/Si epitaxial growth or annealing, hut-to-dome shape transitions were also observed (Floro et al., 1998; Ross et al., 1999; Medeiros-Ribeiro et al., 1998), and these epitaxial islands often adopt faceted surfaces (Mo et al., 1990). It is understood that fully faceted island surfaces are the consequence of cusped energies at certain crystalline surface orientations, that is, surface energy anisotropy. It was proposed that the stability of island arrays is closely related to the arising edge effect from the truly faceted surfaces (Schchukin et al., 1995). However, both recent experimental and theoretic analyses showed that pre-pyramidal islands form with no nucleation barrier, indicating that the truly faceted assumption may no longer be valid and a smooth transition rather than sharp edges between faceted surfaces should exist (Tersoff et al., 2002). Unfortunately, most of the models of heteroepitaxial growth either assume an unfaceted or a fully faceted morphology (Spencer and Tersoff, 1997; Johnson and Freund, 1997; Daruka et al., 1999). To fully understand the island formation and shape transition, an appropriate form of surface energy anisotropy must be included in modeling and theoretical analysis (Zhang and Bower, 2001). There are two challenging issues related to the consideration of surface energy anisotropy: (1) the anisotropy may vary significantly with temperature, alloy composition, and misfit, thus may qualitatively affect the growth morphological evolution and stability as the profiles of surface energy are varied; and (2) faceted surfaces are related to the cusped energies, which normally exhibit sharp changes in surface energy with their surface orientations. This may pose a numerical instability in modeling the evolution of faceted surfaces. Apparently, dependence of surface energy on surface orientation is an unresolved issue, and how the change of surface energy anisotropy affects the island formation and self-organization is another unsolved issue. Here we attempt to construct a quantitative relation between surface energy and surface orientation based on experimental observations and then study how the variation of surface energy anisotropy affects the island formation and self-assembled evolution.

Elastic anisotropy is common in semiconductor materials. For cubic crystalline materials, there are three independent elastic constants \( C_{11}, C_{12} \) and \( C_{44} \), which are related to the Young’s modulus \( E \), the Poisson’s ratio \( \nu \) and the elastic anisotropy strength \( A \) by \( E = (C_{11} + C_{12} - 2C_{12}^2)/(C_{11} + C_{12}) \), \( \nu = C_{12}/(C_{11} + C_{12}) \) and \( A = 2C_{44}/(C_{11} - C_{12}) \). The elastic anisotropy strength can vary from 0.26 for PbTe to 5.2 for InN. For GeSi and Si, it is about 1.6. A first-order analysis of surface roughness of an elastic anisotropic solid has been derived (Gao, 1991). It was shown that the critical wavelength depends on the elastic anisotropy strength. Energetic analysis of the elastic anisotropy effect on the surface roughening mode has been performed (Ozkan et al., 1999). It was shown that the \( \langle 100 \rangle \) roughening mode is more energetically favorable for the heteroepitaxial Ge\(_x\)Si\(_{1-x}\)/Si system. In addition, their annealing experiment using heteroepitaxial Ge\(_x\)Si\(_{1-x}\)/Si system confirms their energetic analysis. Three-dimensional kinetic analysis of the effect of the elastic anisotropy on the island formation and evolution has been performed (Liu et al., 2003). It was shown that elastic anisotropy strongly affects the self-assembly of epitaxial islands: the alignment of epitaxial islands is related to elastic anisotropy strength. For \( A > 1.0 \), the island alignment is along the \( \langle 100 \rangle \) directions. While for \( A < 1.0 \), the island alignment is along the \( \langle 110 \rangle \) directions. This alignment direction is controlled by the directions with the fastest growth wavelength. Hence it is both interesting and practically important to understand the effect of the coupling of elastic anisotropy and surface energy anisotropy on the film surface roughening and island self-assembly.
In this work, finite element simulations are employed to study the surface roughening and island formation and evolution with the consideration of both surface energy anisotropy and elastic anisotropy. Distinctive surface morphologies are obtained by varying the surface energy anisotropy and elastic anisotropy. The relationships between the surface energy and elastic anisotropies and the island formation, shape transition and self-assembly of epitaxial islands are established through simulations. We will show that the calculations considering surface energy anisotropy and elastic anisotropy reproduce many features of experimental results, and elucidate interesting mechanisms underlying the kinetic pathway of island formation and self-assembly.

2. Model formulation

If an elastically anisotropic thin film with lattice spacing $a_f$ is heteroepitaxially grown on an elastically anisotropic substrate with lattice spacing $a_s$, the mismatch strain is defined as $\varepsilon_0 = (a_f - a_s)/a_s$. For simplicity, we neglect the mismatch of elastic properties between the substrate and the film, i.e., the film and substrate have the same elastic properties. Surface mass diffusion and condensation are related to the magnitude of surface chemical potential. For a strained film surface, the surface chemical potential can be written as,

$$\chi = \chi_0 + \Omega \left( \alpha - \kappa \gamma + \nabla_s \cdot \frac{\partial \gamma}{\partial n} \right) \tag{1}$$

where $\chi_0$ is the reference chemical potential, $\Omega$ is the atomic volume of the diffusive atom, $\alpha = \sigma_{ij}e_{ij}/2$ is the strain energy density, $\kappa$ is the mean curvature, and $\gamma$ is the film surface energy, $n$ is the surface unit normal vector, and $\nabla_s$ is the surface gradient operator. It is seen that surface energy anisotropy is included in the chemical potential. In the present treatment, the linear elastic relation between the stress and strain is assumed, i.e., $\sigma_{ij} = C_{ijkl}e_{kl}$, where $C_{ijkl}$ is the component of elastic modulus tensor, $\sigma_{ij}$ is the component of stress tensor, and $e_{kl}$ is the component of strain tensor.

It is known that the growth flux is dependent on the difference between the chemical potential of the vapor phase and that of the film surface. To the first-order accuracy, the growth rate of the thin film surface, $v_g$, is assumed to be proportional to the difference between the chemical potential of the vapor phase, $\chi_0 + \chi_s$, and the surface chemical potential, $\chi$, i.e.,

$$v_g = g(\chi_0 + \chi_s - \chi) \tag{2}$$

where $g$ is a growth parameter, which depends on the sticking coefficient, temperature and the mass of the vapor particle. It is noted that $\chi_s$ is the chemical potential of the vapor phase relative to $\chi_0$, the reference chemical potential.

Both surface diffusion and condensation contribute to the evolution of the film surface. Based on the conservation of mass, the surface evolution rate can be written as

$$v_n = D \nabla_s^2 \chi + g(\chi_0 + \chi_s - \chi) \tag{3}$$

where $v_n$ is the normal velocity, $D = D_s \delta_s/k_B T_s$, $D_s$ is the surface diffusion coefficient, $\delta_s$ is the diffusive layer thickness, $k_B$ is the Boltzmann constant, $T_s$ is the absolute temperature, and $\nabla_s^2 = \nabla_s \cdot \nabla_s$ is the surface Laplacian. Eq. (3) can be written in the following variational form,

$$\int_S v_n \delta v_n \, dA = \int_S (D \nabla_s^2 \chi + g(\chi_0 + \chi_s - \chi)) \delta v_n \, dA \tag{4}$$

where the integration is over the film surface. By assuming a symmetrical condition and applying the surface divergence theorem, we can rewrite Eq. (4) as

$$\int_S v_n \delta v_n \, dA = \Omega \int_S (\alpha - \kappa \gamma)(D \nabla_s^2 \delta v_n - g \delta v_s) - \frac{\partial \gamma}{\partial n} \cdot \nabla_s(D \nabla_s^2 \delta v_n - g \delta v_s) + \frac{\Omega}{\Omega} \delta v_n \, dA \tag{5}$$

This equation may be solved for $v_n$ using the finite element method.

We choose $u$ and $v$ as a set of curvilinear coordinates parameterizing the surface. The surface equation can be expressed by $r(u,v)$. The surface gradient operator can be expressed as (Weatherburn, 1925),
\[ \nabla_s = \frac{1}{H^2} r_1 \left( G \frac{\partial}{\partial u} - F \frac{\partial}{\partial v} \right) + \frac{1}{H^2} r_2 \left( N \frac{\partial}{\partial v} - F \frac{\partial}{\partial u} \right) \]  

where partial derivatives with respect to \( u \) and \( v \) are denoted by the use of the suffixes 1 and 2, respectively; and 
\[ N = r_1 \cdot r_1, \quad F = r_1 \cdot r_2, \quad G = r_2 \cdot r_2 \text{ and } H^2 = NG - F^2. \]

The surface energy is assumed to take the following form:

\[ \gamma(n) = \gamma_0 \left[ 1 - \sum_{i=1}^{V} \Delta \gamma_i \times \exp \left( -\frac{(l_i^2 - l_i^2)^2 + (m_i^2 - m_i^2)^2 + (n_i^2 - n_i^2)^2)}{p_i} \right) \right] \]  

where \( \gamma_0 \) is the maximum value of the surface energy, the surface unit normal direction \( n = \{l, m, n\} \), and \( \Delta \gamma_i \) and \( p_i \) are parameters which can be adjusted to create minima on the surface energy at surface normal directions \( \{l_i, m_i, n_i\} \) for \( i \in (1, M) \), where \( M \) is the number of directions with minimum surface energy. For the GeSi/Si(001) system model, the following faceted surfaces are used: \{100\}, \{501\}, \{311\} and \{15323\} (Ross et al., 1999).

Since GeSi/Si systems follow the Stranski–Krastonov growth mode, it is energetically unfavorable for the substrate to become exposed, that is, the film tends to wet the substrate surface. To model the wetting effect, we have introduced a thin transition layer with varying mismatch strain between the substrate and the fully-strained film. Physically, the transition region can be thought of as a mixed phase of the thin film and substrate, giving rise to the variation of the mismatch strain.

3. Numerical procedure

Since Eq. (5) is very stiff, a finite element method with a semi-implicit Euler scheme is introduced to solve this equation. We perturb the reference surface configuration by a small displacement \( u_n \) along the normal direction of the surface within a small time interval \( \Delta t \). In the forward Euler numerical scheme, we set \( u_n = v_n \Delta t \). The new surface configuration equation is,

\[ r' = r + u_n n \]  

where \( r(u, v) \) and \( r'(u, v) \) are the surface reference configuration and the perturbed configuration, respectively; and \( n \) is the surface normal vector. The mean curvature after the perturbation is (Weatherburn, 1925)

\[ \kappa' = \kappa + \nabla_n^2 u_n + u_n(\kappa^2 - 2K) \]  

where \( K \) is the Gaussian curvature.

After the perturbation, \( \left( \frac{\partial \gamma}{\partial n} \right)' \) can be written as,

\[ \left( \frac{\partial \gamma}{\partial n} \right)' = \frac{\partial \gamma}{\partial n} - \frac{\partial^2 \gamma}{\partial n \partial n} \cdot \nabla_n u_n \]  

Replacing \( \kappa \) in Eq. (5) with \( \kappa' \) and \( \left( \frac{\partial \gamma}{\partial n} \right)' \) with \( \left( \frac{\partial \gamma}{\partial n} \right)' \) in Eq. (10), and rearranging the equation, we can write the semi-implicit scheme as

\[ \int_S u_n \delta v_n + \Delta t \left[ \nabla_n^2 u_n + u_n(\kappa^2 - 2K) \right] q - \Omega \Delta t \left( \frac{\partial^2 \gamma}{\partial n \partial n} \cdot \nabla_n u_n \right) \cdot \nabla_n q \, dA \]

\[ = \Delta t \Omega \int_S (\omega - \kappa)q - \frac{\partial \gamma}{\partial n} \cdot \nabla_n q + g \chi \delta v_n \, dA \]  

where, \( q = D \nabla_n^2 \delta v_n - g \delta v_n \). Eq. (11) may be solved for \( u_n \) by using the finite element method.

We have developed a finite element method for computing the surface evolution of the film (Liu et al., 2003). The geometry of the film surface is specified at time \( t \), our objective is to calculate the shape change of the surface during a subsequent infinitesimal time interval \( \Delta t \). At time \( t \), firstly, we need to calculate the stress and strain distribution along the surface to obtain the strain energy distribution on the surface. The
calculation is based on the linear-elastic and small-strain assumptions. Secondly, we need to calculate the surface curvature based on a rectangular mesh of nine Lagrangian elements on the surface. Finally we need to solve Eq. (11) to obtain surface displacement and a new surface during the time interval $\Delta t$. Based on the configuration at $t + \Delta t$, we are able to calculate the new configuration during a subsequent infinitesimal time interval $\Delta t$. This process is repeated and the surface evolution can be followed.

The finite elements used to solve the surface diffusion equation (Eq. (11)) are the triangular plate bending element. The plate element shape functions are parameterized by the three areal coordinates, $L_1$, $L_2$ and $L_3$. In our calculations, the local coordinates $x, y$ of the plate bending element are used as the curvilinear coordinates. The following relations are used to transform the two coordinate systems:

$$\frac{\partial}{\partial x} = \frac{1}{2A} \left( b_1 \frac{\partial}{\partial L_1} + b_2 \frac{\partial}{\partial L_2} + b_3 \frac{\partial}{\partial L_3} \right)$$

$$\frac{\partial}{\partial y} = \frac{1}{2A} \left( c_1 \frac{\partial}{\partial L_1} + c_2 \frac{\partial}{\partial L_2} + c_3 \frac{\partial}{\partial L_3} \right)$$

where $A$ is the area of the triangular element and

$$b_1 = y_2 - y_3, \quad b_2 = y_3 - y_1, \quad b_3 = y_1 - y_2,$$

$$c_1 = x_3 - x_2, \quad c_2 = x_1 - x_3, \quad c_3 = x_2 - x_1,$$

where $(x_1, y_1), (x_2, y_2)$ and $(x_3, y_3)$ are the nodal coordinates of the triangular element.

All numerical results will be presented in a dimensionless form. Lengths are normalized as $L = L/L_0$, where, $L_0 = \gamma_0/\omega_0$ and $\omega_0$ is the strain energy density on the initially flat (001) surface; the time scale is normalized by $t = t/t_0$, where $t_0 = \gamma_0/(\Omega \omega_0 D)$. In the present simulations, the surface growth rate is chosen as, $g = 0.001L_0/t_0$ and $\nu = 5\Omega \omega_0$.

4. Results

In the present work, the effects of the coupling of the elastic anisotropy and surface energy anisotropy on the surface roughening and island formation and self-assembly have been simulated. In these simulations, the elastic modulus $E$ and the Poisson’s ratio $\nu$ are held fixed, while the elastic anisotropy strength $A$, is varied. In addition, both $\Delta \gamma_i$ and $p_i$ for all the surface orientations with a minimum surface energy are assumed to have the same value. The unperturbed film surface is the (001) surface. For the surface before growth, a random perturbation in the form of Fourier series with random amplitudes and wavelengths is introduced on the film surface to mimic the initial surface roughness. The simulation results are not qualitatively affected by the initial random surface perturbation. Therefore all of the simulations reported here start from the same random surface. The dimensionless length and width of our simulation cells are both 40. The dimensionless substrate thickness is 16. The dimensionless transitional layer thickness is 0.1.

Systematic parametrical studies have been performed to investigate the effects of the elastic anisotropy strength $A$, surface anisotropy parameters $\Delta \gamma_i$ and $p_i$ on the formation and evolution of epitaxial islands. Our simulations show that the formation and morphologic evolution of epitaxial islands are strongly dependent on the anisotropy strength of both surface energy and elasticity. It is found that with an increase in surface energy anisotropy, that is, through an increase in $\Delta \gamma_i$; or with a decrease in $p_i$, the surface shape becomes more faceted and transition between different shapes becomes more difficult. When the elastic anisotropy $A > 1.0$, it is found that the islands are formed predominantly by a breakup of the ripples which are along (100) orientations. This tendency becomes stronger when the elastic anisotropy strength is stronger.

For the case of a weak surface energy anisotropy strength and elastic isotropy, that is, $\Delta \gamma_i = 0.0002$, $p_i = 0.14$ and $A = 1.0$, when the thin film thickness exceeds a certain value, islands form as shown in Fig. 1(a) and (b). Since the islands form through surface roughening, it involves a nucleationless mode without a nucleation barrier (Tersoff et al., 2002). With further growth, island volumes gradually increases as shown in Fig. 1(c). After some of the islands reach a critical volume, it is seen that some larger islands adopt a dome
shape encased by the \{311\} facet surfaces while smaller islands still adopt a spherical cap or cosine-like shape (Fig. 1(d)). This means that the islands adopting the \{015\} hut shape do not appear for this case.

If the surface energy anisotropy strength is increased to a moderate level while the elasticity remains isotropic, for example, for the case with $\Delta \gamma_i = 0.0004$, $p_i = 0.14$ and $A = 1.0$, the \{015\} hut islands form, followed by the roughening and cosine-like island formation as shown in Fig. 2(a) and (b). Island merging occurs after continuing growth, and the resulting larger islands still adopt the \{015\} hut shape as shown in Fig. 2(c). The nucleation of high-angle facet surfaces occurs due to the impingement of the island bases, as indicated by the arrows in Fig. 2(d). Thus both hut shape and dome shape islands can co-exist for this case.

If the surface energy anisotropy strength is strong while the elasticity remains isotropic, for example, for the case with $\Delta \gamma_i = 0.0008$, $p_i = 0.14$ and $A = 1.0$, the \{015\} hut islands form directly during the surface roughening process as shown in Fig. 3(a). These faceted islands grow in a self-similar manner as shown in Fig. 3(b) and (c). Since the \{015\} islands are very stable, no shape transition to high aspect islands occurs in this case (Fig. 3(d)).

If the surface energy anisotropy strength is very strong while the elasticity remains isotropic, for example, for the case with $\Delta \gamma_i = 0.001$, $p_i = 0.14$ and $A = 1.0$, ripples with the \{015\} faceted surfaces form directly.
during the surface roughening process. During the formation of the ripples, the \{015\} faceted islands also form. These faceted islands do not completely break up, but instead connect weakly by ripples. In this case, both hut islands and ripples co-exist. If the surface energy anisotropy strength becomes extremely strong while the elasticity remains isotropic, for example, for the case with $\Delta \gamma_i = 0.0012$, $p_i = 0.14$ and $A = 1.0$, only ripples with the \{015\} faceted surfaces appear. No hut island formation is observed.

For the cases of a weak surface energy anisotropy strength and moderate elastic anisotropy, that is, $\Delta \gamma_i = 0.0002$, $p_i = 0.14$ and $A = 1.6$, ripples and islands forms with a strong alignment along the $\langle 100 \rangle$ directions as shown in Fig. 4(a) and (b). It can be seen that some islands adopt a rounded and non-faceted shape while others adopt the \{015\} facet surfaces. With further growth, island volumes gradually increases and some of the islands start to have a shape transition to adopt a dome shape encased by the \{311\} facet surfaces as shown in Fig. 4(c). From Fig. 4(d), it can be seen that the rounded and non-faceted islands, the square-based and hut-faceted islands, rectangular-based hut-faceted islands and the dome-faceted islands co-exist at this stage.

For the cases of a moderate surface energy anisotropy strength and moderate elastic anisotropy, for example, $\Delta \gamma_i = 0.0004$, $p_i = 0.14$ and $A = 1.6$, ripples and islands form with a strong alignment along the $\langle 100 \rangle$
directions as shown in Fig. 5(a) and (b). It can be seen that only square-based hut islands and rectangular-based hut islands are formed. No rounded and non-faceted islands are observed (Fig. 5(b) and (c)). With further growth, one of the islands undergoes a shape transition from the hut shape into a dome shape (see the arrow in Fig. 5(d)). It is likely that the impingement of the hut-island with its neighboring islands causes the shape transition.

For the cases of a strong surface energy anisotropy strength and moderate elastic anisotropy, for example, \( \Delta \gamma_i = 0.0006 \), \( p_i = 0.14 \) and \( A = 1.6 \), ripples and islands form with a strong alignment along the \([100]\) directions as shown in Fig. 6(a). Similarly to the previous case, only square-based hut islands and rectangular-based hut islands are formed as shown in Fig. 6(b)–(d). With further growth, no shape transition from the hut shape to dome shape is observed. However, it is seen that there is island ripening in which the small square-based hut islands are merged with the elongated islands. For a stronger surface anisotropy strength and the same elastic anisotropy, that is, \( \Delta \gamma_i = 0.0008 \), \( p_i = 0.14 \) and \( A = 1.6 \) the tendency for this transition becomes stronger as shown in Fig. 7(a)–(d). If both surface energy anisotropy and elastic anisotropy are stronger, for example, \( \Delta \gamma_i = 0.0008 \), \( p_i = 0.14 \) and \( A = 4.0 \), this tendency becomes even stronger as shown in Fig. 8(a)–(d). These
Fig. 7. Island cooperative formation and evolution for $\Delta \gamma_i = 0.0008$, $p_i = 0.14$ and $A = 1.6$: (a) formation of $\{501\}$ facet ripples along the soft-directions, [010] or [100]; (b) the elongate-based islands are formed by propagation along [010] or [100] direction; (c) the formation of islands is completed; and (d) the smaller square-based hut islands are merged with the elongated islands. Few hut shape islands exist.

Fig. 8. Island cooperative formation and evolution for $\Delta \gamma_i = 0.0008$, $p_i = 0.14$ and $A = 4.0$: (a) formation of $\{501\}$ facet ripples along the soft-directions, [010] or [100]; (b) the propagation of the island formation along [010] or [100] direction; (c) long base islands are formed; and (d) almost no square hut shape islands exist.

Fig. 9. Island cooperative formation and evolution for $\Delta \gamma_i = 0.0008$, $p_i = 0.20$ and $A = 4.0$. A uniform and regular island array can be formed. (a) $t_\ast = 18.40$; (b) $t_\ast = 20.00$; (c) $t_\ast = 24.00$ and (d) $t_\ast = 46.41$. 
simulations suggest that a combination of a strong surface energy anisotropy and a strong elastic anisotropy may lead to the formation of quantum wire structures.

By changing the magnitude of the surface energy anisotropy and elastic anisotropy, a uniform and regular island array can be formed. For example, the evolution snapshots with $\Delta \gamma_i = 0.0008$, $p_i = 0.20$ and $A = 4.0$ as shown in Fig. 9 exhibits such island arrangement. This result demonstrates that it is potentially possible to fabricate uniform and regular island arrays by tuning the surface energy anisotropy and elastic anisotropy.

5. Discussion and summary

Based on our parametric studies, the variation of the island morphology with surface energy anisotropy parameters for the isotropic elasticity can be schematically described by the phase diagram shown in Fig. 10. The data points denote the present calculation results. It can be seen that depending on $\Delta \gamma_i$ and $p_i$, the different surface morphologies, such as, pure spherical cap (or cosine-like) islands, a mixture of spherical cap and dome islands, pure dome islands, a mixture of dome and hut islands, pure hut islands, a mixture of hut and ripples, and pure ripple structures, can be observed. Interestingly, some of the surface morphologies, for example, pure spherical cap islands, pure hut islands, a mixture of hut and dome islands, pure dome islands, and ripples have already been observed experimentally.

For the SiGe system, since $A > 1.0$, the fastest growth direction is along the $\langle 100 \rangle$ directions, which are also the orientations of the softest elastic stiffness. This result is consistent with the previous energetic analysis (Ozkan et al., 1999) and the experimental results of the Ge$_x$Si$_{1-x}$/Si systems during annealing (Ozkan et al., 1999) and during growth (Mo et al., 1990). Under certain growth conditions, the islands adopt a rectangular base with $\{015\}$ facet surfaces while small islands still maintain a square base (Mo et al., 1990). Under other growth conditions, a transition of a hut shape island into a dome shape was also observed (Ross et al., 1999; Floro et al., 1998; Medeiros-Ribeiro et al., 1998). These results are reproduced by the present simulations under different combination of elastic anisotropy and surface energy anisotropy.

By comparing the cases without elastic anisotropy, for example, Figs. 1–3, with the cases with elastic anisotropy, for example, Figs. 4–6, it is found that inclusion of elastic anisotropy promotes both the formation of hut-faceted islands, and the elongation of hut island bases. The underlying reason is that the elastic anisotropy promotes the alignment of islands along the $\{100\}$ directions. Since some of the $\{510\}$ faceted surfaces can be parallel to one of the $\{100\}$ directions, this alignment makes the formation of the $\{510\}$ hut islands energetically more favorable and the elongation of the hut island bases kinetically more favorable.

![Fig. 10. Schematic phase diagram showing the dependence of surface morphologies on the surface energy anisotropy parameters, $\Delta \gamma_i$ and $p_i$, for $A = 1.0$. Seven different regions are observed: pure spherical cap islands, a mixture of spherical cap and dome islands, pure dome islands, a mixture of dome and hut islands, pure hut islands, a mixture of hut islands and ripples, and pure ripples. The data points denote the present simulation results.](image-url)
From Figs. 3–8, it is found that surface roughening usually starts from some location and then travels like a wave to spread over the entire surface. Thus these surface structures (islands and ripples) are formed through cooperative formation. The possible underlying mechanism is that due to the stress amplification caused by an existing surface structure, the roughening rate at its neighboring region is significantly increased, which facilitates the formation of high-angle faceted surfaces, causing a cooperative formation of surface structures. Such cooperative formation of surface structures has been observed before (Jesson et al., 1996). The present results show that the cooperative formation of surface structures is quite common for films with certain levels of surface energy anisotropy and elastic anisotropy. The underlying reason may be that both surface energy anisotropy and elastic anisotropy exert constraint for the island formation (in terms of shapes and orientations). This constraint may be eased by the cooperative formation.

Although the proposed surface energy functional form (Eq. (7)) is only qualitative in nature, many experimental observations have been reproduced. More importantly, the present parametric studies have demonstrated the strong dependence of island morphologic evolution on both surface energy and elastic anisotropies. This dependence may also explain the rich and diverse phenomena observed in different film systems or in the same film system at different compositions and temperatures. It should be mentioned, however, that a more accurate relation between surface energy and its surface orientation is necessary to better understand heteroepitaxial island growth. Apparently more work is required to quantify this relationship.

In summary, the effects of surface energy anisotropy and elastic anisotropy on the island formation and evolution of a model epitaxial system have been studied. It is shown that the surface energy anisotropy and elastic anisotropy can strongly influence the formation and evolution of epitaxial growth. By changing both the surface energy anisotropy and elastic anisotropy, the diverse surface morphologic patterns can be obtained. This provides additional degrees of freedom to control the island uniformity and regularity.

References


