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Cuboidal-to-pyramidal shape transition of a strained island on a substrate

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ABSTRACT

The stability of a strained cuboidal island deposited on a substrate has been numerically investigated by means of finite element simulations in the case where the structure is submitted to misfit strain resulting from the lattice mismatch between the island and the substrate. In the hypothesis where the surface energy is isotropic, it is found that, depending on the island volume, the formation of a truncated or inverted truncated pyramid can be favored by the misfit strain with respect to the cuboidal shape. A shape diagram is finally provided as a function of the misfit strain and island volume.

The control of the morphological evolution and ageing of patterned surfaces of materials is the topics of intensive research in the physics of surface and materials science because of their numerous potential applications in engineering. For example, the resulting nanostructures developed onto the surface of substrates are involved in a number of electronics and photonics devices. It is now well admitted that the misfit strain resulting from the lattice mismatch at the interfaces between islands, quantum dots or wires and their substrates can be responsible for the morphological change of the nanostructures as well as the formation of defects such as dislocations. One of the consequences of these evolutions is the modification of the electronical, optical or mechanical properties of the devices. For example, it has been observed that Ag islands grown on Si(001) substrate can undergo a transition from square to rectangle shape for a misfit of 6% [1]. Equivalent observations have been reported for Au islands on Mo(111) or Ag(110) substrates. From a mesoscopic point of view, the effect of the misfit strain has been theoretically investigated by Tersoff et al. [1] and others [2–5]. In the framework of linear elasticity theory, the elastic relaxation due to the misfit has been determined using the force monopole approximation that has been found to be efficient for two dimensional (2D) nanostructures for which the strain along the normal direction to the substrate surface in the islands can be considered as constant. Considering thus the surface and step energies and the elastic energy of relaxation, it has been found that beyond a critical volume, an initially two-dimensional island undergoes a morphological transition and evolves from a square to rectangle shape [2]. In the case where the force monopoles point in opposite directions at neighboring steps, a regime where both compact and elongated islands co-exist has been also identified [3]. Likewise, this square-to-rectangle shape transition has been analyzed for vacancy islands on Ge(001) surface due to surface stress anisotropy [4] and the effect of strain on the formation of two-dimensional islands on curved and patterned substrates has been discussed still in the framework of the dipole force approximation [5,6]. Using the dipole-interaction formalism, the elastic energy of a rectangular island on an isotropic substrate has been analytically determined and compared to the one deduced from the monopole approximation and to the energy determined from molecular simulations in the case of Cu/Ni(100) islands [7]. It has been found that both elastic analytical approaches underestimate the critical island size. The formation of pyramids, dome-like and dislocated islands have been intensively studied and for Ge islands grown on Si(100) substrate for example, the different facets have been analyzed as a function of the island size [8] and a shape diagram has been proposed as a function of volume and surface energy for strained islands taking into account steeper facets [9]. The role of strain dependent surface energies on the island formation in the same Ge/Si(100) system has been also investigated combining continuum determination of the strain energy with first-principle calculations of the strain-dependent surface energies [10,11]. Likewise, the coarsening of a distribution of square-based pyramids has been studied and the possibility of preserving the same shape has been discussed [12]. More recently, a shape transition from domes to {111} pyramids has been analyzed as the amount of Ge deposition on pit-patterned Si(001) substrate increases [13]. It has been also found that the kinetic growth modes of islands such as layer-to-layer or faceted growth are strongly correlated to the nonequilibrium composition profiles in strained alloy quantum dots [14]. In particular, the formation of InGaAs dots on GaAs by faceted growth and of GeSi dots on Si by first layer-by-layer growth and then faceted growth has been discussed. GaN/Mg and InGaN/GaN

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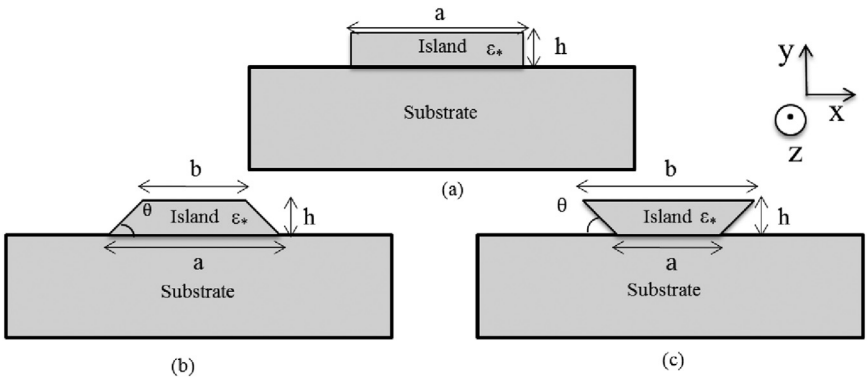

Fig. 1. Strained islands on a substrate represented in the (*Oxy*) plane. (a) Cuboidal island of sides a and height h. (b) Truncated pyramid of height h and lower and upper sides a and b, respectively. (c) Inverted truncated pyramid of height h and lower and upper sides a and b, respectively.

multi-quantum-wells (MQW) have been recently developed [15] using photoelectrochemical wet etching technique where lateral, bottom-up and anisotropic etching have been sequentially used to produce inverted hexagonal pyramids of width 245 nm and height 184 nm. It has been then reported that the equilibrium shape of the islands minimizing the surface energy term is obtained for [0001] Ga-face and exposed $\{10\bar{1}\bar{1}\}$ faces. An angle between the top GaN/Mg surface and the pyramid sidewall has been calculated to be 56.7°. Although the shape is controlled by surface energy through Wulff theorem, it has been finally found that strain is present which modifies the photoluminescence emission of the islands.

The purpose of the present work is to study the effect of the elastic relaxation on the shape evolution of an initially cuboidal island of finite and constant height in the framework of the linear elasticity theory with the help of finite element (FE) simulations. Releasing the constant strain hypothesis of the force monopole approximation [1–3] and considering thus the elastic relaxation of the misfit strain along the normal axis to the substrate surface, the possibility of formation of a truncated or inverted truncated pyramid has been analyzed from an initially cuboidal island, in the hypothesis where the surface energy of the structure is assumed to be isotropic.

An island of initial cuboidal shape of height h and sides a in the (Oxz) plane is considered on the surface of a semi-infinite substrate (see Fig. 1a for axes), where h has been assumed to be a constant in the present work. The truncated and inverted truncated pyramids of same height h and lower and upper sides a and b are displayed in Fig. 1b and c, respectively. In the following, a misfit strain is considered in the island due to the lattice mismatch between the substrate and the island at the interface, such that $\epsilon^*_{xx} = \epsilon^*_{yy} = \epsilon^*_{zz} = \epsilon_*$, with ϵ_* a constant related to the lattice mismatch. The evolution of the island is supposed to occur at constant volume and the surface and step energies are considered to be isotropic such that focus is on the study of the effect of the misfit strain. Neglecting thus the crystallographic effect [1], the total surface energy of the island is determined in the case of the Stransky–Krastanov growth mode where a few layers of the film are assumed to appear before the island. In this case, the interface energy per unit surface γ_i is zero and both surface energies of the upper and lower horizontal surfaces of the island are equal and labeled γ_s. The surface energy per unit surface of the lateral facets is labeled γ_e and, following previous studies [1,2], an angle θ has been introduced to characterize the shape evolution of the island in the (Oxy) vertical plane as:

$$\cot\theta = \frac{a-b}{2h}. \tag{1}$$

In these conditions, the surface energy of the island is found to be [1]:

$$E_s = \left(\frac{\gamma_e}{\cot\theta} - \gamma_s\right)(a^2 - b^2). \tag{2}$$

Introducing the parameter Γ such that:

$$\Gamma = \gamma_e \csc\theta - \gamma_s \cot\theta, \tag{3}$$

it yields:

$$E_s = 2h\Gamma(a+b). \tag{4}$$

It is underlined that the above Eq. (4) of surface energy E_s applies for both truncated pyramids ($b > a$ and $b < a$) but also for the cuboidal island. The next step of this work has been to determine the elastic energy of relaxation due to the misfit strain ϵ_*. Since the height of the nanostructures is not negligible with respect to the other in-plane dimensions, no analytical expression of the elastic energy can be provided to the best of the Authors knowledge and standard finite element calculations have been performed with the help of the commercial software ABAQUS [16]. Following [2], the dimensionless parameter has been introduced:

$$\alpha = \frac{\gamma h}{E_0}, \tag{5}$$

with

$$V_0 = h^3, E_0 = \frac{1+\nu}{(1-\nu)^2}\frac{h^2 E}{2\pi}\epsilon_*^2, \tag{6}$$

where it has been assumed without lost of generality that $\gamma_e = \gamma_s = \gamma$, with E the Young modulus and ν the Poisson ratio of the island. The island and the substrate have been meshed with 4 node tetraedric elements with linear interpolation degree and reduced integration. The numbers of elements for the substrate are typically 25 along the (Ox) and (Oz) directions and 5 along the (Oy) directions. For the refined zone of the substrate in contact with the island, one takes 100 × 100 elements in the interface. For the island, 2 elements along the (Oy) direction and between 13 and 33 elements along the (Ox) and (Oz) directions are considered. It has been checked but not shown that the values of the elastic energy calculated with 2 elements are very close to the ones obtained with 10 elements. In the following, only 2 elements along the vertical direction have been used for optimizing the procedure of elastic energy calculation. The misfit deformation has been mimicked by thermal expansion procedure in the island that is equivalent in the present case to the eigenstrain method, and the substrate has been considered as clamped at its bottom horizontal surface. It is emphasized that the elastic calculation has been performed neglecting the effect of the wetting layer. The elastic coefficients have been taken to be $E = 117$ GPa and $\nu = 0.343$ for silicon material and the elastic energy E_e has been determined in the structure for different dimensionless volumes