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# Size selection of strained islands during Stranski–Krastanov growth

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ABSTRACT

The formation of isolated circular islands submitted to misfit strain has been theoretically investigated on the surface of a thin wetting layer of constant thickness deposited on a substrate by calculating the chemical potential of the island atoms. It is found that the island size selected by the misfit strain depends on the difference between the shear moduli of the islands (and wetting layer) and the substrate. An analytical expression for the island radius is derived from the first order development in the shear modulus difference.


## 1. Introduction

The heteroepitaxial growth of thin films on substrates has been intensively studied from both experimental and theoretical points of view for many years, since it has been proved to be a promising way to produce self-assembled and self-organized nano-structures (see [1–5] and the references therein). In particular, the effect of strain on the island size distribution has been widely investigated in the framework of surface physics and continuum mechanics [6–9]. During the Volmer–Weber (V–W) growth mode, the islands directly grow on the surface of the substrates while the islands develop on a wetting layer during the Stranski–Krastanov (S–K) growth mode. For V–W growth, it has been demonstrated that the elastic interaction between two-dimensional (2D) strained islands influences the island size distribution during the coarsening processes with and without island motion [10]. Likewise, for three-dimensional (3D) islands, it has been found that, due to island edges, a stable shape is selected against coarsening for the islands, leading to self-assembled patterns of uniform sized structures [11]. When the island–island interaction is strong, the effect of film coverage on the island size has been also characterized by the same author for strained and non-strained islands. For an isolated island, the stress induced by the lattice mismatch at the film-substrate interface for heteroepitaxy as well as the stress due to the substrate surface anisotropy for homoepitaxy have been found to be responsible for a transition from square to elongated shape as the size of the islands increases [12–14].

When a wetting layer is present, a phase diagram has been theoretically constructed which predicts the different growth modes, the density and size of dislocation-free islands as a function of the film thickness and misfit strain [15]. The elastic interaction between misfit nanostructures has been also investigated through finite element calculations and the sign of this interaction has been found to be dependent on the island sizes [16]. The effect of the neighbor islands on the wetting in S–K growth has been numerically investigated, the wetting decreasing with increasing island density [17]. The influence of strain on the surface energies in the island formation for Ge/Si(100) system has been characterized combining first-principles and continuum calculations [18]. The effect of strain on the Ge/Si growth mode has been investigated in stacked layers and the influence of the decrease of the Ge critical thickness in the upper layers has been characterized on the increase of the island size and height [19]. Likewise, the effect of anisotropic strain, surface energy and surface diffusivity has been theoretically studied on the self-organization of island patterns on surfaces [20].

In this work, the size selection of islands growing on the surface of a strained wetting layer has been theoretically investigated from a chemical potential calculation in the regime where the dislocation-free islands grow separately onto the surface of the film whose thickness is assumed to be constant. The effect of shear modulus difference between the film and the substrate is characterized.

## 2. Modeling

A 2D circular island of radius $R$ and height $h_{is}$ is considered on the surface of a thin layer of thickness $h_f$ submitted to misfit strain due to a coherent interface between the film and a semi-infinite substrate (see Fig. 1a). The Young's modulus and Poisson's ratio are labeled $G_f$ and $\nu_f$ for the island and the film and $G_s$ and $\nu_s$ for the substrate, respectively. The island growth is studied assuming that the film thickness is constant, i.e. the film does not grow vertically and the islands are too far apart to interact. The film and island are assumed to be free of

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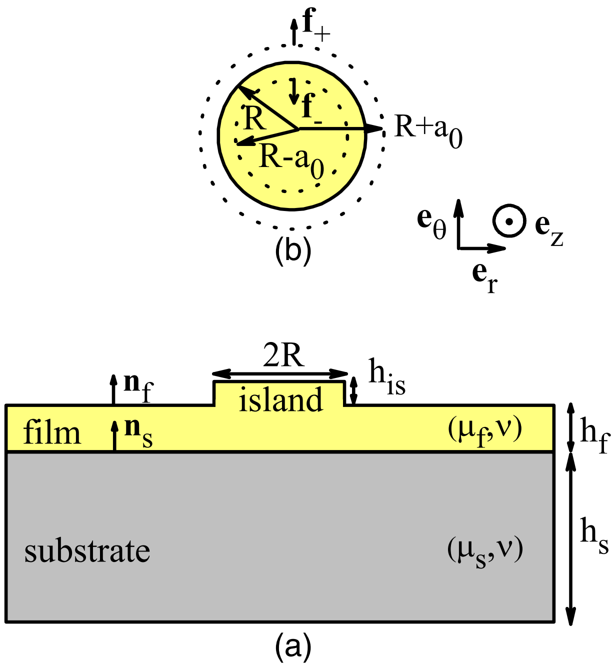


**Fig. 1.** (a) A 2D circular island of radius $R$ and thickness $h_{is}$ lying onto the surface of a thin film of thickness $h_f$ deposited on a substrate of thickness $h_s >> h_f$. (b) Top view of the island: to model the elastic relaxation, two distributions of force monopoles $\mathbf{f}_+$ and $\mathbf{f}_-$ are introduced onto the surface of the film at $R_+ = R + a_0$ and $R_- = R - a_0$, respectively.

dislocations and the intrinsic surface strain is not considered. In the following, taking $\nu_s = \nu_f = \nu$, one focuses in the framework of linear and isotropic elasticity, on the shear modulus effect on the island shape selection due to misfit strain. In this hypothesis, it is assumed that the island growth is governed by the chemical potential of the island atoms defined as [10,11]:

$$\mu_c = \frac{s}{2\pi R}\frac{d\mathcal{F}_{tot}}{dR}, \tag{1}$$

where $s$ is the area occupied by one atom and $\mathcal{F}_{tot}$ the total energy associated with the island:

$$\mathcal{F}_{tot} = \mathcal{F}_{su} + \mathcal{F}_{el}, \tag{2}$$

with $\mathcal{F}_{su}$ the surface energy and $\mathcal{F}_{el}$ the elastic relaxation energy. For the 2D circular island on the film free-surface, assuming the surface energies of the film and the island are identical [21], the surface energy term yields:

$$\mathcal{F}_{su} = 2\pi R\gamma, \tag{3}$$

with $\gamma$ the edge energy per unit length. The elastic relaxation energy has been determined using Boussinesq's force formalism [22–24,12]. Indeed, for 2D strained structures, it has been demonstrated that when the strain does not vary along the $(Oz)$ perpendicular direction to the film surface, the elastic effect can be modeled using distributions of force monopoles along the island perimeter. In the case of an isolated circular island, the following procedure has been used [25]. It is assumed that the elasticity problem can be solved considering two distributions of force monopoles $\mathbf{f}_- = -\delta(r - R + a_0)f_0\mathbf{e}_r$ and $\mathbf{f}_+ = \delta(r - R - a_0)f_0\mathbf{e}_r$, with $\delta$ the Dirac delta function, $\mathbf{e}_r$ the unit radial vector and $a_0$ a cut-off length of the order of the lattice parameter (see Fig. 1b). The force intensity per unit length $f_0$:

$$f_0 = 2G_f\frac{1+\nu}{1-\nu}\frac{\delta a}{a_s}h_{is}, \tag{4}$$

depends on the misfit strain $\delta a/a$, the island height $h_{is}$ and the thin film elastic constants $G_f$ and $\nu$, with $\delta a$ the lattice mismatch between the film and the substrate and $a_s$ the lattice parameter of the substrate. In this hypothesis, the elastic energy variation is given by $\mathcal{F}_{el} = -\frac{1}{2}\varepsilon_{el}^{in}$ where $\varepsilon_{el}^{in}$ is the elastic energy interaction between both distributions $\mathbf{f}_-$ and $\mathbf{f}_+$. The elastic energy relaxation due to the island thus writes:

$$\begin{aligned}\varepsilon_{el} &= -\frac{1}{2}\varepsilon_{el}^{in} = \frac{1}{2}\int_S \mathbf{f}_-\mathbf{u}^{+f}dS \\ &= -\pi f_0(R-r_0)u_r^{+f}(R-r_0,0),\end{aligned} \tag{5}$$

where $\mathbf{u}^{+f}$ is the elastic displacement on the surface of the film due to the $\mathbf{f}_+$ distribution and $S$ the film surface. This 2D axi-symmetrical problem of elasticity has been solved in the cylindrical coordinate system $(r,\theta,z)$ for a given circular distribution of force monopoles $\mathbf{f}_\pm = \pm\,\delta(r - R_\pm)f_0\mathbf{e}_r$, introducing a bi-harmonic function $\phi_\pm^i$ which satisfies [26–28],

$$\Delta\Delta\phi_\pm^i(r,z) = 0, \tag{6}$$

with $\Delta$ the Laplacian operator, $R_\pm = R \pm a_0$ and $i = f$ for the film and $i = s$ for the substrate. Eq. (6) has been solved using the method of integral transform [26–28]. Taking the Hankel transform of zero order for $\phi_\pm^i$:

$$G_\pm^i(\zeta,z) = \int_0^{+\infty} r\phi_\pm^i(r,z)J_0(\zeta r)dr, \tag{7}$$

it yields:

$$G_\pm^i(\zeta,z) = \left(A_\pm^i + B_\pm^i z\right)e^{+\zeta z} + \left(C_\pm^i + D_\pm^i z\right)e^{-z\zeta}, \tag{8}$$

with $J_n$ the Bessel function of the first kind of nth order. The elastic displacement $\mathbf{u}^{\pm,i}$ and stress tensor $\overline{\overline{\sigma}}^{\pm,i}$ can be derived from the $\phi_\pm^i$ function using the linear elasticity theory. The different coefficients $A_\pm^i$, $B_\pm^i$, $C_\pm^i$ and $D_\pm^i$ have been determined writing the following boundary conditions for the epitaxially strained thin film on its semi-infinite substrate: zero normal pressure on the film free-surface, mechanical equilibrium and non-gliding condition at the film/substrate interface:

$$\overline{\overline{\sigma}}^{\pm,f}(r,0)\cdot\mathbf{n}_f = \mathbf{f}_\pm, \tag{9}$$

$$\overline{\overline{\sigma}}^{\pm,f}\left(r,-h_f\right)\cdot\mathbf{n}_s = \overline{\overline{\sigma}}^{\pm,s}\left(r,-h_f\right)\cdot\mathbf{n}_s, \tag{10}$$

$$\mathbf{u}^{\pm,f}\left(r,-h_f\right) = \mathbf{u}^{\pm,s}\left(r,-h_f\right), \tag{11}$$

with $\mathbf{n}_f$ and $\mathbf{n}_s$ the unit normal vector of the film free-surface and film/substrate interface, respectively (see Fig. 1b). Assuming that $\phi_\pm^s$ takes finite values when $z \to -\infty$, one sets $C^{\pm,s} = D^{\pm,s} = 0$. The system of Eqs. (9)–(11) has been solved, the expressions of the other non-zero constants being not displayed in this paper, and the elastic energy term has been found to be:

$$\begin{aligned}\varepsilon_{el} &= \pi(1-\nu)\frac{f_0^2}{G_f}\left(R^2-a_0^2\right) \\ &\times\int_0^{+\infty}\frac{\chi_1}{\chi_2}e^{-2kh_f}J_1(k(R-a_0))J_1(k(R+a_0))dk,\end{aligned} \tag{12}$$