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Circular-to-elliptical-to-circular shape transitions of strained islands

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ABSTRACT

The shape transition of a one-layer thick strained island deposited on a semi-infinite substrate has been theoretically investigated from an energy variation calculation. It is found that depending on the misfit strain, the initially circular island may become unstable beyond a critical size and can evolve toward an elliptical shape. As the surface of the island increases, another transition is expected to occur which consists in the ellipse splitting into two identical circular islands of smaller size. A shape diagram is finally displayed for the island as a function of the misfit strain and island surface and a scenario of nanostructure evolution is discussed.

1. Introduction

The study of the size and morphological evolution of nanostructures developed onto the surfaces of solids is a long-standing problem in surface physics and materials science since their physical and chemical properties depend on the arrangement of atoms [1–4]. In this way, it is now well admitted that the structure of quantum dot patterns are strongly dependent on the coarsening which can in turn modify the properties of the nanostructures and, as a consequence, their applications in engineering fields [5]. Various strain relaxation mechanisms can also modify the properties of the nanostructures. Indeed, the misfit strain resulting from the lattice mismatch between the substrate and the islands may be relaxed through the formation of dislocations, alloying or shape modification. In particular, it has been found that an initially strained square-like island can undergo a shape transition beyond a critical size and can evolve toward a rectangular shape (or quantum wire) [6–8]. This shape transition has been then characterized for vacancy islands in the presence of surface stress anisotropy [9] or when the misfit strain is anisotropic [10] and of different sign [11] along both in-plane directions [10,11]. The effect of substrate curvature has been also investigated [12]. It has been found for example that in the case of Ge islands deposited on curved silicon-on-insulator substrates, the stress and composition in the structure are modified as well as the alloying when the kinetic effects are important. Likewise, it has been theoretically demonstrated that the formation of islands on the top of an apex or the bottom of a valley can be trigged by the substrate curvature (and the strain relaxation) [13]. The case of island formation on a sawtooth pattern has been also considered [14]. Likewise, the island shape transition in Si(001) homoepitaxy has been investigated with the help of a low-energy electron microscopy and the effect of intrinsic surface stress anisotropy on the elliptical-to-football shape transition has been characterized [15].

In this Paper, the shape evolution of an initially two-dimensional circular island deposited onto the free surface of a semi-infinite substrate and submitted to misfit strain has been theoretically studied. The transitions from a circular to an elliptical shape and from the elliptical to new circular shapes have been characterized as a function of the island surface and misfit strain.

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2. Modeling and discussion

An initially one-layer thick or two-dimensional (2D) island is considered on a semi-infinite substrate (see Fig. 1 for axes). The radius of the circular island in Fig. 1 (a) is labeled R and the radii along major and minor axes in Fig. 1 (b) are labeled a and b for the ellipse, respectively. The transition from the circular to elliptical shape has been studied, assuming the surface of the island is constant, i.e. $\pi ab = \pi R^2$. In the hypothesis where for the one-layer thick island the misfit strain is constant in the direction of the axis perpendicular to the free surface [6], the elastic energy relaxation has been calculated using the force monopole approximation with Green function formalism of the isotropic and linear elasticity theory [6,7,16-18]. Considering thus the following force monopole distribution along the perimeter of the island $\mathbf{F} = E\varepsilon_0 a_0 \mathbf{n}$, where ε_0 is the misfit strain related to the lattice mismatch between the island and the substrate, $\mathbf{n}$ the normal of the island boundary and a_0 the height of the one-layer island, the relaxation elastic energy is given by [7–11]:

$$E_{elas} = -\frac{1}{2}\int\int \mathbf{u}(\mathbf{r}_1, \mathbf{F}_2(\mathbf{r}_2))\mathbf{F}_1(\mathbf{r}_1)d\mathbf{r}_1 d\mathbf{r}_2, \tag{1}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the boundary coordinates, $\mathbf{F}_1$ and $\mathbf{F}_2$ are the force evaluated at $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively, and $\mathbf{u}(\mathbf{r}_1, \mathbf{F}_2(\mathbf{r}_2))$ is the elastic displacement field at $\mathbf{r}_1$ induced by the force $\mathbf{F}_2$ evaluated at $\mathbf{r}_2$. This displacement field is defined as:

$$\mathbf{u}\left(\mathbf{r}_1, \mathbf{F}_2(\mathbf{r}_2)\right) = \frac{1+\nu}{\pi E}\left(\frac{1-\nu}{r}\mathbf{F}_2(\mathbf{r}_2) + \frac{\nu}{r^3}\mathbf{r}_1\left(\mathbf{F}_2(\mathbf{r}_2)\cdot\mathbf{r}_1\right)\right). \tag{2}$$

Introducing the elliptical coordinate system, Eq. (1) has been written as:

$$\begin{aligned} E_{elas} = &-\frac{(1+\nu)F^2}{4\pi E} \times \int_0^{2\pi} d\theta_1 \int_{\theta_1+\theta_0}^{\theta_1-\theta_0+2\pi} d\theta_2 (1-\nu) \\ &\times \frac{(a^2-b^2)\sin^2\frac{\theta_1+\theta_2}{2} - (a^2+b^2)\sin^2\frac{\theta_2-\theta_1}{2} + b^2}{\sin\frac{\theta_2-\theta_1}{2}\sqrt{(a^2-b^2)\sin^2\frac{\theta_1+\theta_2}{2} + b^2}} \\ &+ \nu\frac{-a^2b^2\sin\frac{\theta_2-\theta_1}{2}}{\left(b^2+(a^2-b^2)\sin^2\frac{\theta_1+\theta_2}{2}\right)^{\frac{3}{2}}}, \end{aligned} \tag{3}$$

with $F = E\varepsilon_0 a_0$, $\theta_0 = \frac{a_0}{R} << 1$ the cut-off angle, θ_1 and θ_2 two angles characterizing the positions of the forces $\mathbf{F}_1$ and $\mathbf{F}_2$ of the distribution, respectively, E the Young modulus and $\nu = 0.3$ the Poisson ratio of the island. It is underlined at this point that the integral defined in Eq. (3) has been analytically determined in the following to the leading order in θ_0. In order to characterize the first circular-to-elliptical shape transition, the following ellipse parameter e has been introduced:

$$a = R\sqrt{1+\left(\frac{e}{R}\right)^2} + e, b = R\sqrt{1+\left(\frac{e}{R}\right)^2} - e, \tag{4}$$

with $e << R$. Developing thus the relaxation elastic energy given in Eq. (3) to the fourth order in e and to the leading order in θ_0, it yields:

$$\begin{aligned} E_{el} = &-E_{el}^0(1-\nu)\left[2\pi R\ln\left(\frac{R}{a_1}\right)\right. \\ &\left. + \frac{3\pi}{2R}\ln\left(\frac{R}{a_2}\right)e^2 - \frac{15\pi}{32R^3}\ln\left(\frac{R}{a_4}\right)e^4\right] + \Theta(e^5), \end{aligned} \tag{5}$$

with $E_{el}^0 = (1+\nu)\varepsilon_0^2 a_0^2 E/\pi$ and the a_1, a_2 and a_4 the cut-off lengths defined as:

$$a_1 = \frac{a_0}{4}\exp\left(\frac{2-\nu}{1-\nu}\right), a_2 = \frac{a_0}{4}\exp\left(\frac{14-11\nu}{3(1-\nu)}\right), \tag{6}$$

$$a_4 = \frac{a_0}{4}\exp\left(\frac{(46-31\nu)}{15(1-\nu)}\right). \tag{7}$$

The first term in the above expression of energy displayed in Eq. (5) corresponds to the elastic energy of a circular island of radius R [8], the second and third ones being related to the elliptical shape. In order to characterize the stability of the island, a surface energy term has also to be considered. Assuming that in the Stranski-Krastanov growth regime, the film wets the substrate before the islands appear, the surface energy term E_s reduces to the step energy [6]. It yields:

$$E_s = \gamma P, \tag{8}$$

with γ the line energy assumed to be isotropic and P the island perimeter defined as:

$$P = 2\int_0^{\pi}\sqrt{\left(\frac{dx}{d\theta}\right)^2 + \left(\frac{dy}{d\theta}\right)^2}d\theta, \tag{9}$$

where the island perimeter is described by $x = a\cos\theta, y = b\sin\theta$ in the elliptical coordinate system. Developing Eq. (9) to the fourth order in e gives:

$$E_s = 2\pi R\gamma + \frac{3\pi\gamma}{2R}e^2 - \frac{15\pi\gamma}{32R^3}e^4 + \Theta(e^5). \tag{10}$$

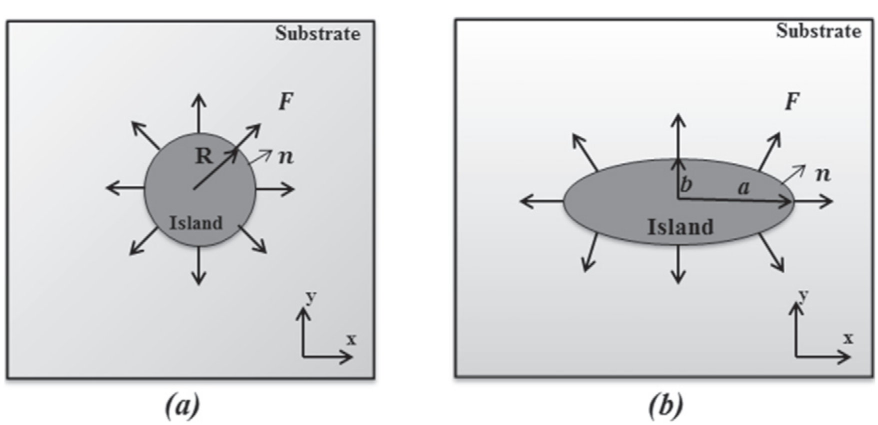

Fig. 1. Schematic top view of strained islands grown on a semi-infinite substrate. (a) Circular shape of radius R. (b) Elliptical shape of radii a and b.