# Theory of equilibrium shape of an anisotropically strained island: Thermodynamic limits for growth of nanowires

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Using continuum elastic theory, we show that strain anisotropy removes the shape instability existing for an isotropically strained island. An anistropically strained island has always an anisotropic shape, elongating along the less-strained direction and adopting a narrow width in the more-strained direction. The sign of strain makes only a quantitative difference without changing the qualitative island shape. Our study establishes thermodynamic limits for growing nanowires with anisotropically strained islands.

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The study of equilibrium shape of strained island on surface is of both scientific interest and technological significance. Equilibrium shape of a strained (stressed) two-dimensional (2D) island gives a direct manifestation of surface thermodynamic properties including surface step energy and surface stress;[1–3] growth of strained 2D and three-dimensional (3D) islands provides also a unique method for fabrication of nanowires on surface.[4–12]

Equilibrium theory of island shape has been established for 2D[1] and 3D[4] islands on surface under *isotropic* strain. Most noticeable, strain induces a spontaneous shape instability in the growth of 2D (3D) island on surface:[1,4] there exists a critical size, controlled by competition between isotropic step (surface) energy and strain energy, below which the island adopts an isotropic shape (such as a square for 2D island) and above which it adopts an anisotropic shape (such as a rectangle). The strain-induced shape instability has also been shown for 3D inclusions in bulk.[13,14]

The strain induced island shape elongation has been applied for growing nanowires on surface.[4–12] One problem associated with growing wires using isotropically strained island is that it may elongate along either $x$ or $y$ direction with two energetically degenerate shapes.[1,4] To make all the wires oriented along the same direction, an idea has been proposed[9,10] to grow island that is strained in one direction but strain-free in the other (orthogonal) direction so that it grows only along the strain-free direction. However, such a scenario is hard to find with a real materials combination between the islands and substrate.

Most wires have been grown with islands that are generally *anisotropically* strained on surface. A typical system is rare-earth metal silicide nanowires[8–10] grown on Si(001), which has attracted much attention because of its application in integrated circuits. However, existing theories[1–4,11–14] have focused mostly on *isotropically* strained islands. Although the effect of strain anisotropy has been speculated[4,9] and a special case of 2D island anisotropy with the same stress magnitude but opposite signs has been considered,[1] a general theory of equilibrium shape of 2D or 3D islands under *anisotropic* stress/strain is still lacking. This creates a gap in the understanding of the experimental growth of nanowires using anistropically strained islands, such as those silicide wires.[8–10]

Several pending questions are especially important with regard to growth of nanowires: (1) Will an anisotropically strained island, like an isotropically strained island, exhibit a shape instability? (2) When an island is anisotropically strained, will it be only stable along the less-strained direction with one energy minimum, or will it be also metastable along the other more-strained direction with a local energy minimum? (3) How does the island shape anisotropy depend on strain anisotropy? (4) For given strain anisotropy, does the sign of strain (i.e., tensile or compressive in both directions versus tensile in one direction but compressive in the other direction or vice versa) matter?

Here, we perform a general theoretical analysis of equilibrium shape of 2D island under *anisotropic* strain (or stress). We demonstrate that the existence of strain anisotropy removes completely the island shape instability associated with isotropically strained island. As long as the strain is anisotropic, there will be only one energy minimum along the less-strained direction at all island sizes without the second local minimum in the orthogonal more-strained direction. Thus, thermodynamically, the island prefers always to grow along the less-strained direction, and its aspect ratio increases with increasing island size. For a given island size, the larger the strain anisotropy is, the larger the island aspect ratio is. The sign of strain makes only a quantitative difference, without changing the island shape behavior qualitatively.

We analyze the equilibrium shape of a 2D island under biaxial *anisotropic* strain, using continuum elastic theory, similar to the previous analysis for a 2D island under *isotropic* strain.[1] Consider the general case of a rectangular island of length $a$ and width $b$ strained along the $x$ and $y$ direction, respectively, with $\varepsilon_{xx}$ and $\varepsilon_{yy}$, as shown in Fig. 1. The strain introduces elastic force monopoles ($F_x$ and $F_y$) along the island boundary, whose magnitude is proportional to the magnitude of strain and the island height and whose direction follows the respective sign of strain (tensile versus compressive) in each direction.

The island strain energy is calculated as[15]

$$E_{\text{strain}} = -\frac{1}{2}\int\int d\vec{x}d\vec{x}'\vec{F}_1(\vec{x})\cdot\vec{u}[\vec{x},\vec{F}_2(\vec{x}')], \tag{1}$$

where, $\vec{u}[\vec{x},\vec{F}_2(\vec{x}')]$ is the displacement at $\vec{x}$ induced by a force at $\vec{x}'$. Let $\vec{r}=\vec{x}-\vec{x}'$:

 

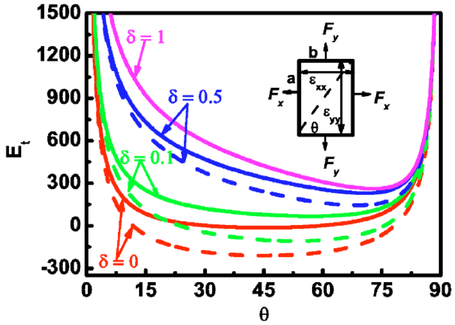


FIG. 1. (Color online) Total energies ($E_t$) of a strained 2D rectangular island (see inset) vs $\theta = \tan^{-1}(a/b)$ for different strain anisotropies ($\delta$). The island size is chosen to be smaller than the critical size associated with the isotropically strained island. Solid curves are for strains having the same sign in the two directions (both compressive or tensile); dashed curves are for strains having different signs (compressive along $x$ and tensile along $y$ direction; or vice versa).

$$\vec{F}_1(\vec{x}) \cdot \vec{u}\,[\vec{x},\vec{F}_2(\vec{x}')] = \frac{1-\nu^2}{\pi\mu}\frac{\vec{F}_1 \cdot \vec{F}_2}{r} + \frac{\nu(1+\nu)}{\pi\mu}\frac{[\vec{F}_1 \cdot \vec{r}][\vec{F}_2 \cdot \vec{r}]}{r^3}, \tag{2}$$

where $\mu$ is Young's modulus and $\nu$ is Poisson's ratio. For a rectangular island, the first term in Eq. (2) arises only from the interaction between parallel or antiparallel force monopoles on the two opposite island sides ($a$-to-$a$ or $b$-to-$b$). The second term includes also the interaction between orthogonal force monopoles at the two neighboring sides ($a$-to-$b$ or $b$-to-$a$), describing the Poisson effect that compression (tension) in one direction leads to tension (compression) in the orthogonal direction.

Integration of Eq. (1) along the island boundary gives

$$\frac{E_{\text{strain}}}{E_s} = PG_1(c,\gamma) - P \times 2(1-\nu)G_2(c,\gamma)\ln\frac{D}{a_0} + PO(\frac{a_0}{D}). \tag{3}$$

Here, using the same notations as in Ref. 1, $E_s = [(1+\nu)/(2\pi\mu)]F_x^2$. $P = 2(a+b)$ is the island boundary length. $c^2 = a/b$ is the island aspect ratio (shape anisotropy). $\gamma = F_y/F_x = \varepsilon_{yy}/\varepsilon_{xx}$ is the ratio of strain in the two directions. $D = \sqrt{ab}$ is the island size. $a_0$ is a cutoff length.[1] The term $O(a_0/D) = 4[(1-\gamma+\gamma^2)\nu - (1+\gamma^2)]a_0/D$ is very small and can be neglected as in Ref. 1, because generally $D \gg a_0$. $G_1$ and $G_2$ are given by

$$G_1(c,\gamma) = \frac{1}{2(c+\frac{1}{c})}\left(2(1-\nu)\left(c\ln\frac{\sqrt{c^2+\frac{1}{c^2}}+c}{\sqrt{c^2+\frac{1}{c^2}}-c} + \frac{\gamma^2}{c}\ln\frac{\sqrt{c^2+\frac{1}{c^2}}+\frac{1}{c}}{\sqrt{c^2+\frac{1}{c^2}}-\frac{1}{c}} - 2c\ln\frac{c}{e} - 2\frac{\gamma^2}{c}\ln\frac{1}{ce}\right)\right.$$
$$\left. + 4\left\{c\gamma^2 + \frac{1}{c} - \left[1+\gamma^2 - 2(1-\gamma+\gamma^2)\nu\right]\right\}\sqrt{c^2+\frac{1}{c^2}} + 2(1-\gamma)(c\gamma - \frac{1}{c})\right) \tag{4}$$

and

$$G_2(c,\gamma) = \left(c + \frac{1}{c}\right)^{-1}\left(c + \frac{\gamma^2}{c}\right). \tag{5}$$

Note that setting $\gamma = 1$, $G_2(c,\gamma) = 1$ and $G_1(c,\gamma)$ reduces to $G(c)$ in Ref. 1; the Eqs. (3)–(5) return to solutions of isotropically strained island. Here, we consider only the case of isotropic boundary (step) energy, the total energy of the island is then $E_t = E_{\text{strain}} + PE_b$, where $E_b$ is the boundary energy per unit length.

We have determined the equilibrium island shape via total-energy minimization, as a function of island size ($D$) and of strain anisotropy ($\delta$). To facilitate our discussion, we define strain anisotropy as $\delta = 1 - |\gamma|$, with $0 \leqslant \delta \leqslant 1.0$. For $\delta = 0$, strain is isotropic, i.e., zero or no strain anisotropy; for $\delta = 1.0$, strain anisotropy is the largest, as the $y$ direction is strain free. The strain in the $x$ direction, i.e., $E_s$ is kept fixed.

Figure 1 shows the total energy $E_t$ as a function of $\theta = \tan^{-1}(a/b)$, calculated using the parameters of, $E_b/E_s = 3.02$. The island size ($D/a_0 = 50$) is chosen to be smaller than the critical size for shape instability ($D_c/a_0 = 113$ for $\gamma > 0$, and $D_c/a_0 = 209$ for $\gamma < 0$) associated with the isotropically strained island, i.e., for $\delta = 0.0$, the island adopts an isotropic square shape with a single minimum at $\theta = 45°$, as shown in Fig. 1.

As long as $\delta \neq 0.0$ (no matter how small it is), the energy minimum always shifts away from $\theta = 45°$ to a larger value. Thus, the existence of strain anisotropy leads always to an anisotropic shape, removing the shape instability (i.e., the

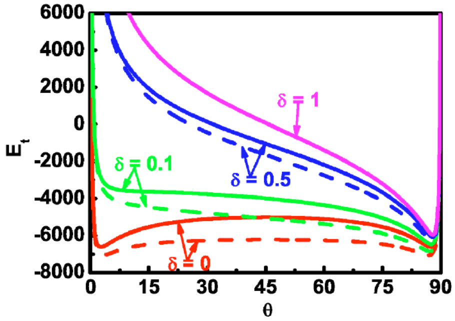


FIG. 2. (Color online) The same plot as Fig. 1, except that the island size is chosen to be larger than the critical size associated with the isotropically strained island.

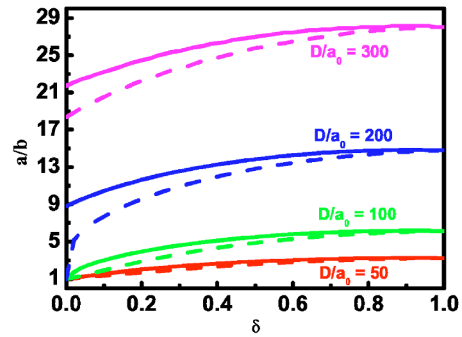


FIG. 3. (Color online) Calculated optimal (equilibrium) island aspect ratio ($a/b$) vs strain anisotropy ($\delta$) for four different island sizes of $D/a_0=10$, 100, 200, and 300. The notations are the same as in Fig. 1.

existence of a critical size) possessed by an isotropically strained island. As the energy minimum shifts to the $\theta>45°$ side, the island will always elongate along the less-strained $y$ direction. The energy minimum continues to move further to larger $\theta$ with increasing $\delta$. So, for a given island size, the larger the strain anisotropy, the larger the island aspect ratio, i.e., a more elongated island along the less-strained direction.

For a given strain anisotropy, $\delta$ (except for $\delta=1.0$ when strain is zero along the $y$ direction), there may be different signs of strains: both compressive or tensile along $x$ and $y$ direction versus compressive along $x$ and tensile along $y$ direction or vice versa. Figure 1 shows that for the same $\delta$, the energies of islands under strains of different signs (dashed curves) are always slightly lower than those under strains of the same sign (solid curves). This results from the Poisson effect described by the second term in Eq. (2), the interaction between orthogonal force monopoles on the neighboring island sides.[16] The overall strain is effectively smaller and hence the energy is lower when the island is under different signs of strain, because compression in one direction compensates tension in the other direction and vice versa. However, the sign of strain does not qualitatively change the picture.

Figure 2 shows the same plot as Fig. 1 for the case of an island size ($D/a_0=300$) chosen to be larger than the critical size of the shape instability associated with the isotropically strained island. So, for $\delta=0.0$, there are two degenerate energy minima, one with $\theta>45°$ and the other with $\theta<45°$ (the two lowest curves in Fig. 2). This means that at this size, the isotropically strained island would elongate along either $x$ or $y$ direction with equal probability.

For $\delta\neq 0.0$, however, no matter how small it is, there is only one energy minimum at the far side of $\theta>45°$. This indicates that for any anisotropically strained island, it will only be thermodynamically stable by elongating along the less-strained $y$ direction. There does not exist a metastable shape along the more-strained $x$ direction. For large island size, the effect of elongation along the less-strained direction is even very pronounced with a very small strain anisotropy of $\delta=0.1$ with $\theta>85°$.

The fact that the island is only thermodynamically stable to elongate along one direction, the less-strained direction, without a metastable state in the orthogonal direction has an important practical implication. It implies that to align the nanowires along the same direction, from the thermodynamic point of view, one may not need to find a materials combination with very large strain anisotropy, in particular strained only in one direction and strain-free (lattice matching) in the other direction as suggested earlier.[9,10] A small strain anisotropy with 10% difference in the two directions may still be sufficient to drive wires to grow along one direction, at the thermodynamic limit. This provides a greater degree of flexibility in choice of materials for growing nanowires via elongation of anisotropically strained islands.

Same as Fig. 1, Fig. 2 shows that for the same strain anisotropy ($\delta$) the energies of islands under strains of different signs (dashed curves) are always slightly lower than those under strains of the same sign (solid curves), with energy minima at slightly different positions. In general, as indicated by the positions of energy minima, the larger the strain anisotropy is, the larger the island aspect ratio is. This is more clearly illustrated in Fig. 3, which shows island aspect ratio ($a/b$) as a function of strain anisotropy ($\delta$) for several island sizes ($D/a_0=10$, 100, 200, and 300). For $\delta=0$, small islands, such as $D/a_0=10$ and 100, have $a/b=1.0$, as they are smaller than the critical size of shape instability and maintain an isotropic shape; large islands above the critical size, such as $D/a_0=300$, have $a/b>1.0$, becoming elongated. For $\delta\neq 0.0$, islands of all sizes have $a/b>1.0$, elongating along the less-strained $y$ direction.

For all $\delta$, the aspect ratio of those islands under the different signs of strains (dashed curves in Fig. 3) is smaller than that of those islands under the same sign of strains (solid curves). This difference decreases with increasing $\delta$. As $\delta$ increases, the island becomes more elongated so that the interaction between force monopoles on the two long opposite sides becomes dominant, while the interaction between orthogonal monopoles on the two neighboring sides, which gives rise to the difference, becomes negligible.

One interesting phenomenon occurs at $\delta=0$ for $D/a_0=200$. The island under the different signs of strains ($y$ intercept of $D/a_0=200$ dashed curve) has an isotropic shape with $a/b=1.0$, while the island under the same sign of strains ($y$ intercept of $D/a_0=200$ solid curve) has an anisotropic elongated shape with $a/b\sim 9.0$. This reflects that the sign of strain changes the critical size of shape instability for the isotropically strained island, which again can be understood

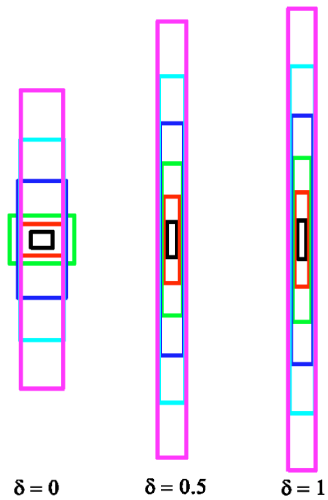


FIG. 4. (Color online) Evolution of equilibrium island shape with increasing island size for islands under different strain anisotropy of $\delta=0$, 0.5, and 1.0.

by the Poisson effect discussed earlier. Although the magnitude of strain is the same in two directions, the overall strain is effectively smaller for the island under different signs of strains, leading to a smaller critical size, as the critical size decreases with increasing strain.[1,4]

Previous studies[1,4] have shown that an isotropically strained island elongates only above the critical size, beyond which it continues to elongate with a fixed width. In contrast, an anisotropically strained island elongates at all sizes. In Fig. 4, we show the evolution of equilibrium island shapes with increasing island size for strain anisotropy of $\delta=0$, 0.5 and 1.0. Under isotropic strain ($\delta=0$), the island first grows in its size isotropically, then elongates along one direction while shrinks in the other, later it elongates with a fixed width.[4] Under anisotropic strain ($\delta=0.5$, and 1.0), the island has initially an elongated shape with a narrow width. It then grows preferentially along the less-strained direction while its width converges quickly to a fixed value. In general, the larger the strain anisotropy is, the longer and narrower a nanowire will grow.

Although, for simplicity, we have performed analysis for 2D islands, the results we obtain can be readily applied to 3D islands for growth of nanowires. In fact, those 3D islands used for growing nanowires must be constrained kinetically with a fixed height, so effectively they can be treated as quasi-2D islands.[1,4] Without height constraint, a 3D island would always in principle grow its height to more effectively relax strain, rather than elongating laterally on surface.[1,4]

Our study is especially relevant to growth of rare-earth silicide nanowires,[8–10] which are generally under anisotropic strain and are of great technological significance. We show that anisotropic strain may help improve orientational order of nanowires, driving them to grow along the less-strained direction. The wires may grow with uniform width distribution. The sign of strain makes only a quantitative difference. Longer and narrower nanowires can be grown by choosing a materials combination with larger strain anisotropy. These are all in good qualitative agreement with existing experimental results.[5–10]

In summary, we present a theoretical study of equilibrium shape of anisotropically strained 2D islands, establishing thermodynamic limits for growing nanowires on surface. We note that while thermodynamically strain anisotropy may work favorably for fabricating nanowires, kinetic factors have also to be taken into account. Future work is needed to investigate the competition between thermodynamics and kinetics, in order to obtain a more complete understanding of growing nanowires with anisotropically strained islands.

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