Existence of shallow facets at the base of strained epitaxial islands

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(Received 9 April 2002; published 23 October 2002)

We generalize a previous analysis of equilibrium shapes of strained epitaxial islands, to include the possibility of facets of smaller slope both above and below facets of greater slope. We find that the lower shallow facet exists exactly when the upper shallow facet does. Thus the conclusions of our previous analysis are unaffected, except that the actual island shape is modified by the presence of an additional facet in certain cases.

DOI: 10.1103/PhysRevB.66.132104 PACS number(s): 81.10.Aj, 68.35.Bs

In a previous paper,[1] we studied the equilibrium shape of fully facetted Stranski-Krastanow islands that are under stress due to epitaxial misfit with the substrate. We found that there is generally a first-order transition with increasing island volume, as new steeper facets are introduced. We did not consider the most general possible shape, but rather assumed that the facets become increasingly steep near the edge of the island, as in Fig. 1(a).

Here we consider a more general shape, Fig. 1(b), which allows for the possibility of a shallow facet below the steep facet. We find that such a lower shallow facet (LSF) will be present in exactly those cases where the upper shallow facet (USF) is present. Aside from the presence of the LSF, the qualitative conclusions of Ref. 1 are unaffected. However, the actual island shape (whenever both shallow and steep facets are present) is as in Fig. 1(b) rather than Fig. 1(a). This is consistent with experimental observations of lower shallow facets even in annealed islands.[2] In addition, the position of some boundaries in the ''phase diagram'' will move, but without changing any qualitative features of the phase diagram.

Because the significance of our analysis is primarily qualitative in any case, we have not actually recalculated the phase diagram for the generalized shape. Instead, we use analytical arguments to extend our previous results.

We begin by considering the shape 2 or 2′ assumed previously [Fig. 1(a)], and ask whether the energy would be lowered by introduction of a lower shallow facet, as in Fig. 1(b). Using Eqs. (1)–(3) of Ref. 1, the change in the total island energy by the introduction of an infinitesimal LSF can be written, up to linear order in facet size, as

$$\Delta E=(\Gamma_1-\Gamma_2/s)L. \tag{1}$$

Here L is the length of the LSF projected onto the plane of the surface. Other notation is as in Ref. 1: $\Gamma_n=g_n(1+s_n^2)^{1/2}-g_0$ is the extra surface energy per projected area for facet n ($n=0$ corresponds to the surface orientation, $n=1$ to the shallow facet, and $n=2$ to the steep facet); and g_0, g_1, and g_2 are the surface free energies per unit length for the respective facets. (This assumes a Stranski-Krastonow island, i.e., an island atop a wetting layer of the same material, so that the surrounding surface also has surface free energy g_0.) Also, $s=s_2/s_1$ is the relative slope of the steep and shallow facets.

The energy change in Eq. (1) arises from the change in surface energy due to the introduction of the LSF. In addition, there are terms of order L^2 (aside from any logarithmic corrections) arising from the elastic relaxation energy change at the edges of the LSF, and from the rearrangement of the existing facets. (This rearrangement of the existing facets is necessary to keep the island volume fixed while introducing the infinitesimal LSF. It gives no energy change up to linear order in L, because the chemical potential is the same for each existing facets in the initial shape.)

From Eq. (1), one can see that the introduction of an infinitesimal LSF will decrease the island free energy if and only if $\Gamma_1-\Gamma_2/s<0$. This condition for the existence of the LSF is exactly the same as the condition, derived in Ref. 1, for the existence of the upper shallow facet. Thus, the LSF exists exactly when there is an USF present in the island, so the number of distinct equilibrium shapes is unchanged. However, in Fig. 3 of Ref. 1, the shapes [shown in Fig. 1(a) here] should be replaced with those in Fig. 1(b).

In addition, the position of the boundaries in the island-shape ''phase diagram'' will move, but without changing any qualitative features of the phase diagram. Specifically, in Fig. 3 of Ref. 1, those boundaries that are straight horizontal lines are unaffected, but the left-side boundaries of regions 2 and

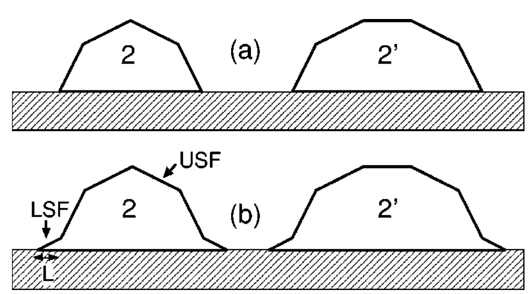

FIG. 1. (a) Island shapes having both shallow and steep facets, as assumed in Ref. 1. Labels 2 and 2′ are from Ref. 1. (b) Shapes 2 and 2′ as they should be, including LSF.

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$2'$ will be shifted to the left. (The magnitude of the shift of the 1-2 boundary goes smoothly to zero at the 1-2-3 ''triple point'', and that of the 0-$2'$ boundary goes smoothly to zero at the 0-$2'$-$3'$ ''triple point'', as does the size of the LSF; so the 1-3 and 0-$3'$ boundaries are unaffected.)

Finally, we note that these arguments apply directly to three-dimensional (3D) islands, when the steep and shallow facets lie in the same azimuth. For example, on a (001) surface, if a strained island of some material exhibits only $\langle a0n \rangle$ and/or $\langle b0n \rangle$ facets, or only $\langle aan \rangle$ and/or $\langle bbn \rangle$ facets, the same criteria for the shape would apply. We suspect that the criterion also applies more generally, as in the case of SiGe islands on Si (001), which exhibit $\langle 105 \rangle$ and $\langle 113 \rangle$ facets, as well as facets of lower symmetry. However, we do not at present have a rigorous treatment of the general 3D problem.

[1] I. Daruka, J. Tersoff, and A.-L. Barabási, Phys. Rev. Lett. **82**, 2753 (1999).

[2] A. Rastelli, M. Kummer, and H. von Känel, Physica E **13**, 1008 (2002).