Energies of Strained Surfaces and Barrierless Formation of Strained Islands

In a recent Letter [1], Tersoff, Spencer, Rastelli, and von Känel (TSRK) suggested that the barrierless formation and faceting of SiGe islands on Si(100) can be consistently explained by making an assumption that the surface energy $\gamma(\theta)$ has an additional minimum at $\theta \neq 0$. We comment here the following points: (i) This minimum in the surface energy need not be postulated and is not restricted to the SiGe system; rather, it is a general feature of a strained crystal surface; (ii) models invoking a stepped morphology can explain the barrierless formation of strained islands, contrary to the TSRK statement; (iii) the attribution of the island surface as thermally rough by TSRK requires a more rigorous treatment.

(i) We have shown recently [2] that the elastic interaction between the strain field of an atomic step and a uniform strain field reduces the line energy of steps to negative values. Creation of steps on a strained surface lowers the surface energy until a limit due to step-step repulsion is reached. As a result, the surface energy $\gamma(\theta)$ has a minimum at an angle $\theta_0 \neq 0$. An analytical expression and the numerical estimates for θ_0 are given in Ref. [2]. Such behavior of $\gamma(\theta)$ is a general feature of a strained crystal surface. In particular, for the material parameters of the SiGe system, we have found that $\theta_0 \approx 11°$, in good agreement with the slope of the (105) facet. TSRK assume that $\gamma(\theta)$ have two equally deep minima, one at $\theta = 0$ and another one at $\theta_0 \approx 11°$. In contrast, our model [2] gives a minimum at θ_0 but a local maximum at $\theta = 0$.

(ii) TSRK argue that the step-based models of island formation cannot be applied because of the thermal roughening of the surface. We note first, before we discuss the roughness, that there is no conflict between predictions of continuous and step models. We illustrate this in Fig. 1 by calculating the equilibrium island shapes in a two-dimensional model, similar to TSRK, but using the chemical potentials μ_n of the interacting steps. Specifically, we find a solution of the set of equations $\mu_n = \text{const}$ for a given volume and a given island height (number of steps) N and then determine the island energy as a function of N. The islands drawn in the left panel are the ones which minimize the energy. The discrete calculation removes the problem of corners which TSRK have to resolve by introducing an additional corner term. Our energy plot has, in contrast to TSRK, only one minimum at each volume.

(iii) TSRK characterize the island surface as thermally rough, based on a room-temperature STM image. The island itself is only several atomic steps in height. Observation of this island means that the height fluctuations are small compared with the island height and, hence, are comparable with a step height. If so, the surface still can be treated in terms of surface steps

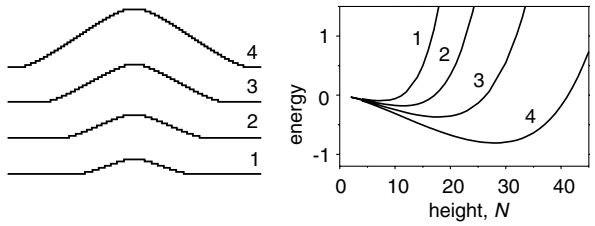

FIG. 1. Equilibrium shapes (left) and energies (right) of strained islands calculated with the model of interacting steps. The stepped island surface is visible in the left panel. The volume of each island in the sequence 1 to 4 is two times larger than the previous one.

even if the steps are not clearly seen on the STM image. The island surface roughness observed by TSRK is notably larger than, say, the roughness of an unstrained Si(001) surface, but, in our opinion, this is not sufficient to make a definitive conclusion if the surface is thermally rough or not. If the (001) surface is rough, as suggested by TSRK, then the (105) surface would be rough as well, since first the thermal roughening of the high-index facets proceeds at lower temperatures and then the roughening of low-index facets takes place at higher temperatures. These contradict the observation of the (105) facets of strained islands.

TSRK speculate that the decrease of the line energy of steps under compressive stress could lead to a lowering of the thermal roughening temperature and result in an atomic-scale roughness. In our opinion, the formation of three-dimensional islands itself is a process of kinetic roughening which proceeds below the thermal roughening transition temperature when the compressive strain decreases the line energy of steps. The presence of individual islands, rather than an undulated surface, is due to the material deficit when a thin strained layer, deposited on the wetting layer in the Stranski-Krastanow growth, is redistributed. We suggest that the faceting of the islands can be qualitatively described by the step-step repulsion which restricts the surface slope.

The theory of strained islands is far from being complete. In our opinion, the step model can provide better insight into the island energetics and kinetics without making additional assumptions of the TSRK model.

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